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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.

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material for publication to the Editorial Office at the IERC address above.

SAM WEISSMAN WINS THE GOLD

It gives us very great pleasure to report that the Gold Medal of the International EPR (ESR) Society has been awarded to Dr. Samuel Isaac Weissman, Professor Emeritus of Chemistry at Washington University in St. Louis, Missouri, USA. Professor Weissman, known to most of us as "Sam", will receive the award in a formal presentation ceremony and celebration during the annual International EPR Symposium at Denver in the last week of July, 1995. The next issue of the EPR Newsletter will feature an account of this event.



Professor Weissman was born in South Bend, Indiana, USA, on June 25, 1912. He attended Chicago public schools and received his undergraduate and graduate education at the University of Chicago, receiving his Ph.D. in 1938. His study of light absorption and fluorescence by europium (III) in solution proved to be a pioneering contribution to the understanding of metal ion solvation. As a postdoctoral fellow at Berkeley with G. N. Lewis, Weissman continued to investigate the absorption and emission of light by molecules. Aspects of his work on intramolecular energy transfer took on added significance decades later in helping to explain laser action. He was involved in the recognition of the triplet state and demonstrated that the singlet-triplet transition has electric dipole character. During this period he also developed the selection rules, independently developed by McClure, that govern the birth of a photoexcited triplet state.

With the entry of the United States into World War II, Weissman resigned his National Research Council fellowship in early 1942 and became involved in the Manhattan Project in Berkeley through his suggestion that it should be possible to separate uranium isotopes photochemically. In the absence of lasers this brilliant idea could not be successfully implemented in the 1940's, but it provides an example of how far ahead of his time Weissman's ideas have been. He moved to Los Alamos in 1943 and became a group leader in the Chemistry and Metallurgy Division. It is remembered that under circumstances that were most trying, he had the cooperation and admiration of his co-workers as a result of both his

professional and personal qualities. Sam Weissman came to Washington University in 1946 where he and a group of young Turks including Lindsay Helmholz, Joseph Kennedy, David Lipkin, Herbert Potratz and Arthur Wahl, founded a modern chemistry department. In fact, it is the work in the area of magnetic resonance that Weissman has carried out at Washington University that has made the greatest impact.

He performed the first definitive EPR experiments on stable cation and anion free radicals. For example, he was the first to obtain proton hyperfine splittings, in this instance on the naphthalene radical anion. Independently, he and Harden McConnell discovered the linear relationship between hyperfine coupling constants and spin density. This is perhaps the most useful concept in the analysis of high resolution EPR spectra. Weissman's radical anion work led him to verify experimentally several fundamental aspects of molecular orbital theory, such as the pairing theorem. He measured hyperfine interactions in corresponding radical cations and anions and found equal distributions of spin density, as predicted theoretically.

He has also had a strong interest in the chemistry of radical anions and cations. Sam Weissman developed some of the first methods for measuring by EPR and NMR spectroscopic techniques the rates of electron transfer reactions. Simultaneously with his experimental work he produced the theoretical expressions that permit electron transfer rates to be derived from EPR spectra. In addition to mono radicals Weissman has made pioneering contributions to the study of other paramagnetic species, including biradicals and triradicals. He and Gerd Kothe were the first to prove the existence of a tri-radical using low frequency EPR. Also, with Jim Norris, he was the first to measure the rotational diffusion of triplet state biradicals using EPR line broadening theory. This work was among the first experimental verifications of the theory of stochastic processes by Kubo. He is also credited as being the first to recognize the electron dipole-dipole interaction as the fundamental cause of triplet state anisotropy that broadens the EPR spectra of randomly oriented triplet states. This had prevented the observation of triplet states by EPR spectroscopy until Clyde Hutchinson, by observing triplet molecules oriented in host single crystals, controlled the spectral broadening caused by the dipolar interaction that Weissman pointed out.

Sam Weissman is also associated, together with his Washington University colleagues Jonathan Townsend and Richard Norberg, with the first observation of liquid-phase electron-nuclear double resonance, ENDOR, the experiment having been performed by Alf Cederquist and developed in his dissertation. Liquid-phase ENDOR, now accessible via commercial instrumentation, is invaluable in many fields of investigation including photosynthesis.

While Sam Weissman is now an emeritus professor, he is more vigorous than most scientists half his age. He remains active in several fields of fundamental importance. In the past ten years he pioneered the study of photoexcited triplet states by time-resolved EPR spectroscopy and was also among the first to use electron spin-echo spectroscopy to study photoexcited triplets. He has designed experiments to establish exciton transfer in model systems composed of closely spaced aromatic rings. Recently, he and Sloop have performed transient EPR without applying microwave or radio frequency radiation to the samples.

It would be wrong not to include among Sam Weissman's scientific achievements the teaching, the training, the encouragement, and the inspiration that he has provided to those around him, whether they be undergraduates, graduate students, postdoctoral fellows or faculty colleagues. Weissman's wonderfully glowing interest and enthusiasm for science, his deep understanding and the clarity of his explanations, his patience with everyone but himself, his warm gentle sense of humor, his humility - all these attributes make him one of the strongest intellectual influences on all who know him. This influence continues - he works in the lab every day with undiminished insight and vigor that is the envy of those forty years his junior. As always he is ready to listen, encourage and help - a great and compassionate scientific leader. For Sam, science has been its own reward, and he has never sought honors for himself. He has given so much to science and scientists, however, that it is most appropriate for his distinguished career and his greatness as a human being to be recognized by the Gold Medal of the EPR society.

Peter Gaspar, Professor of Chemistry
Washington University, St. Louis, MO

LEV BLUMENFELD WINS THE SILVER

We are privileged to announce that Dr. Lev Blumenfeld of the Russian Academy of Sciences, Moscow, has won the IES Silver Medal for his distinguished contributions in EPR related to Medicine and Biology. An award presentation ceremony will be held during the International EPR Symposium at Denver in the last week of July, 1995. The next issue of the EPR Newsletter will feature an article about Dr. Blumenfeld and a report on the award presentation.

FROM THE EDITOR

Future issues: The next issue of the Newsletter will contain the annual information from our database - listings of your EPR colleagues with addresses, affiliations, telephone, Fax, E-mail information, and interests. If you know of anyone we have missed who should be included, or if you know of any corrections that should be made to our list before publication, please notify us immediately.

The IES Awards Committee begins its work in January, so please send your nominations for awards before the end of the year! See "IES Affairs" below for details.

R. Linn Belford

◆ **IES AFFAIRS** ◆
**ANNOUNCEMENTS AND
 REPORTS FROM THE INTER-
 NATIONAL EPR SOCIETY**

From the President —

I am writing this whilst the memory of another remarkable scientific meeting is in my mind. This was the Chianti conference on spin relaxation held in San Miniato, Italy, between Pisa and Florence. I am tempted to say that it was not worth attending, so that those of us who were lucky enough to have been there can keep it to ourselves in future years, but the reverse is true. It was scientifically exciting, particularly in its 50/50 mixture of ESR and NMR, held in a beautiful place, and very remarkable for its social programme. I only hope that the feet of the ladies I danced with have since recovered from being stepped on!

We held a meeting of IES members who attended the Chianti meeting. This is something I like to do at conferences, for the essence of the IES is that it is your Society and exists to serve you. I want always to hear comments on our operation, suggestions for change, and criticisms where they are due. These are invaluable to us, as we try to run a truly international society which depends upon input from all over the world. An inconsiderate action or a lack of action, or an ill-considered remark from any of us in office can cause disaffection without our realising it, and we always prefer to know of our shortcomings, and to correct them. The meeting went very well and Bob Clarkson was asked, upon his return to Illinois, to thank Linn Belford and Becky Gallivan, particularly, for all the work they do on our behalf.

As time rolls on I am continually surprised to discover that some of my colleagues in EPR/ESR reach retirement, although that special form of retirement for the scientist which means that they will actually go on working as hard as

ever, but with perhaps more time now available for research. This year three major scientists, all of whom have made real contributions to their own fields, have reached this stage. I am fortunate that I know them all well, have enjoyed their company for long periods, and regard them all as personal friends. They are John Weil (Canada), Bert de Boer (Netherlands) and Les Sutcliffe (UK), and I am sure that all our members will want me to wish them well on their behalf on their retirements. John and Bert have made significant contributions to the setting up and running of the Society whilst Les has always worked hard to publicise and widen the appreciation of research in magnetic resonance.

Talking of retirement reminds me that it is now only a year before my period of office, and that of my fellow officers, comes to its end, and David Greenslade is, in fact, to give up being Treasurer at Christmas. We are starting to think about our successors, but this should not be in the control of a small self-perpetuating group, but rather should involve everyone. I shall be pleased to receive any nominations that you might make.

The hectic conference round next takes me to Sydney for two meetings, EPR-95, which will largely be a meeting under the auspices of the IES, although completely organised and run by our Australian colleagues, and the ISMAR meeting, in which we are also strongly involved. I am greatly looking forward to my first trip "down under", and to returning to the UK via Fiji and Hawaii. It is a hard life being a scientist!

Keith McLauchlan.

Awards

Important: Nominations for awards for the coming year are due January 1, 1996. We repeat here the Society's award policies: Awards are not restricted to IES members, but the committees may take membership into account when deciding on the award winners. Agreement has been reached between the British and Russian Groups and ourselves to co-operate in the award of the Bruker and Zavoisky Prizes and our Gold Medal Award each year, with each group invited to make input into the selection of each, but with the final choice left to each group. The area of research interest is to rotate between the groups each year, with the loosely-interpreted categories, chemistry, physics and instrumentation, and biological sciences (including medicine), these are meant to be interpreted liberally and not to be restrictive.

In the coming year (1996), the IES Gold Medal award will be in Physics and/or Instrumentation, the Bruker in Chemistry, and the Zavoisky in Biology and/or Biological Sciences. Prof. Larry Berliner, continuing Chairman of the Gold Award committee, will welcome nominations for this.

Gold Medal: 1996 Gold Medal, recognizing benchmark contributions to EPR spectroscopy in physics and/or instrumentation. Send nominations to Prof. Larry Berliner.

Silver Medals: One each in the general areas of Chemistry, Physics/Instrumentation, and Biology/Medicine. To propose names, please send your suggestion(s), or preferably full nomination(s), to the appropriate Silver Awards Sub-committee(s): *For Physics and Instrumentation* - Jim Hyde, Chair; John Pilbrow, George Feher, & Jan Stanowski. *For Chemistry* - Bruce Gilbert, Chair; N. Hirota, Jim Bolton & Kev Salikhov. *For Biol./Medicine* - Harold M. Swartz, Chair; Marjeta Sentjurc, Hideo Utsumi & Tadeusz Sarna.

Young Investigator Awards: One Young Investigator award each year; "young" is defined as less than 7 years since the Ph.D. degree. Awards for 1994 and 1995 will be reported in the next issue of the Newsletter. Before the end of 1995, send nominations for 1996 award to Prof. Keith McLauchlan.

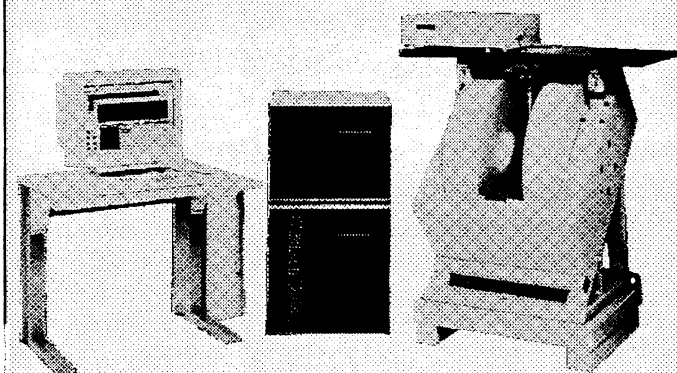
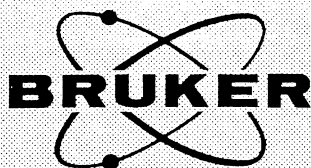
Fellows of the Society

In accord with a proposal made, and accepted, in an unofficial IES business meeting held at the 1994 International EPR Symposium at Denver, your Society has created Fellowships of the Society to recognise truly outstanding contributions and achievements in electron

paramagnetic/spin resonance among these scientists (hopefully, IES members) who are either retired or are close to retirement. The highest international standards are to be applied to the recognition of those worthy of this distinction, and their formal connection with the Society will enhance its own image. Nominations for consideration by the Committee are to be sent in confidence to Keith McLauchlan by January 1, 1996.

From the Treasurer

The financial situation of the society is not bad, although some care is needed in future expenditure. The last two years need to be taken together, and then it can be seen that our expenditure has exceeded our income by about \$2000. Some of this, however, is because of the previous commitments to celebrate the Zavoisky 50th anniversary and send representatives to similar events. Membership fees provide the main base. Commercial sponsorship is also substantial, and we believe that it can and should be significantly expanded. If any member sees any opportunities being missed for raising funds, please let one of the officers know.



The BRUKER worldwide group of companies are proud to be a PATRON of the International EPR Society. For information on products and to determine the sales and service representative for your country, contact Dr. Dieter Schmalbein, BRUKER Analytische Messtechnik, Division IX - EPR, D-76287 Rheinstetten, am Silberstreifen, Germany. Telephone: 49-721-5161-141; FAX: 49-721-5161-237

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Treasurer's Financial Report:

Accounts of the Society for 1994:

INCOME:	1994	1993
Membership fees:		
Collected by S.S.E.	\$25.00	\$3,607.00
by C.F. (note 1)	\$10,530.70	\$6,007.77
Sub-Total	\$10,455.70	\$9,614.77

Industrial Sponsorship

Collected by S.S.E.	- nil -	\$1,100.00
by C.F.	\$6,512.50	\$3,400.00
Sub-Total	\$6,512.50	\$4,500.00

Interest

Collected by S.S.E.	\$78.52	\$323.25
Total Income	\$17,046.72	\$14,438.02

EXPENDITURE:

University of Illinois (Newsletter/database) (note 2) (staff costs, supplies and services)		
S.S.E.		\$4,879.88
C.F.	\$19,355.34	\$2,080.59
Sub-Total	\$19,355.34	\$6,960.47

Denver Meeting (S.S.E.)

Workshop proceedings :		\$418.19
Medal award fees/banquet:	\$1826.53	\$1,013.44
50th Anniversary Dinner		
Complimentary tickets:	\$216.00	
Medical expense for attendee	\$53.99	
Bank Charges		
(SSE- note 3)	\$16.00	\$377.99
Treasurer postage	\$30.00	\$151.00
Travel Bursaries	\$250.00	\$1,450.00
Travel Expenses:		
to Committee Members		
representing the society:	\$1204.22	
to secretariat:	\$ 278.50	

Total	\$23,230.58	\$10,371.09
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RESERVES:

Brought forward from	1993	1992
	\$22,355.89	\$18,288.96
Excess of Income over Expenditure	\$-6,184.58	\$4,066.93

Total	\$16,177.33	\$22,355.89

This was held:		
S.S.E.	\$1,991.00	\$17,007.70
C.F.	\$14,180.33	\$5,348.19

Notes:

1. Funds during this period were held by the former treasurer, Prof. Sandra S. Eaton, in a Denver account identified by her, by U.S. treasurer Dr. Chris Felix in a Wisconsin account, and lesser funds in the U.K. in sterling by myself, which are detailed below. A very small fund is held in Australia by Professor John Pilbrow, and a Russian fund of small dollar value by Prof. Lebedev.
2. Owing to the transfer of duties, there was a delay in paying the University of Illinois. Thus, some items are deceptively large as they include 1993 payments.
3. Transfer of funds can cause large charges if members do not use checks or draughts drawn on U.S. Banks when paying from outside the U.S.A.

U.K. ACCOUNT:

Income:	1994	1993
Membership fees	£1198-00	£941-50
Fee for mailing list	£ 113-86	
Interest on bank account	£4-25	£1-11

	£1316-11	£942-61

EXPENDITURE:

Travel Award	£170-65	
Transfer to U.S.A.(S.S.E)	£346-91	
Expenses: Travel for President	£609-30	
Postage etc.,	£17-00	

	£626-30	£517-56

RESERVES:

Brought forward	£553-83	£128-78
Excess of Income over expenditure	£689-81	£425-05

Total (pounds sterling)	£1,243-64	£553-83

Submitted by David J. Greenslade, Treasurer
University of Essex, Dept. Chem. & Biol. Chem.
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THE COMPUTER CORNER*Edited by Philip D. Morse II, Keith P. Madden,
Graeme Hanson, and Richard Cammack*

The EPR Computer Corner is a regular feature of the EPR Newsletter. It is managed and edited by Reef (Philip D., II) Morse (reef@xenon.che.ilstu.edu), Graeme Hanson (graeme@cmr.uq.oz.au), Keith Madden (MADDEN@marconi.rad.nd.edu), and Dick Cammack (udbc033@hazel.cc.kcl.ac.uk). Items for this column may be sent to any of the above authors. Submissions may be edited for publication.

EPR on the Internet1) EPR List server

People wishing to join an EPR-related discussion list can do so as follows:

Send the single word SUBSCRIBE to epr-list-request@xenon.che.ilstu.edu and you will be automatically placed on the list. You will receive verification of subscription, usually within one or two minutes.

Send messages to epr-list@xenon.che.ilstu.edu. These will be posted to the other subscribers on the list immediately. You will also receive a copy of your posting which confirms that your posting has been sent out. If you want to obtain information about the list, send those requests to epr-list-request@xenon.che.ilstu.edu. Please don't send information requests to the message address.

If your address changes, or you no longer receive mail from the list, please contact me at reef@xenon.che.ilstu.edu and I will make the appropriate changes (you can do this yourself if you want, but I'll be glad to do it for you).

2) EPR on World Wide Web

A number of Web pages specifically for dealing with EPR-related topics have been established across the world. The Illinois EPR Research Center has set up a Web page which will allow access to all the other EPR web pages. The IERC Web home page can be accessed by <http://ierc.scs.uiuc.edu>. Near the bottom, you will find a category "Other EPR Sites", under which is a self-explanatory

list of links to other EPR WWW sites. Click on any line in this list to open the corresponding EPR home page. At this writing, 12 sites were listed (see Yang Fann's discussion later in this column); probably, there will be more by the time you receive this issue!

The IERC (ierc.scs.uiuc.edu) and Illinois State University (xenon.che.ilstu.edu), in cooperation, both maintain anonymous ftp servers which include vendor demonstration programs (xenon), public domain software (ierc), and Rich Cammack's software data base.

3) How to obtain World Wide Web browsers

Browsing these web sites is quite simple if you have a Macintosh, Windows, OS/2, or UNIX PC (Linux works extremely well), or other UNIX machines. These run variants of either Mosaic (available through the National Center for Supercomputing Applications at University of Illinois; connect by anonymous ftp to <ftp.ncsa.uiuc.edu>) or Netscape (an educational version of Netscape is available for free, a commercial version is also available; anonymous ftp to <ftp.netscape.com>). Lacking these tools makes "browsing the web" difficult. However, a text-based web browser is available called Lynx. Lynx has most of the features of Mosaic and Netscape, but without the graphics. Also, Lynx can be quite useful to those who must connect to the Internet through a modem (passing graphics by modem is one of the most time-consuming processes in web-browsing activities). Lynx and DosLynx can be obtained via anonymous ftp to www.ukans.edu and is in the /pub/lynx and /pub/DosLynx (make sure you use proper upper and lower case) directories. Our thanks to Jean Standard, Illinois State University Department of Chemistry, for help in finding these anonymous ftp sites.

New Commercial Software Demonstrations on the Anonymous Ftp Server at ISU (xenon.che.ilstu.edu)

Xenon is a repository for commercial EPR software. Currently, the software offerings of two vendors is available in the directory [anonymous.demos]. Scientific Software Services has had its software described in the newsletter in the past. For this issue, we will focus on new simulation software written by L.I. Antsiferova and E.V. Valova at the Institute of Chemical Physics in Chernogolovka. They can be reached by E-mail at Antsif@icp.ac.ru. —

EPR Simulation Software

Our program calculating ESR spectra for nitroxides in microheterogeneous media is based on the stochastic Liouville equation which includes the general dynamic model for inhomogeneous systems. In this model, the random molecular rotations are considered as the stochastic process characterized by dynamic parameters which also change by sporadic jumps between two sets of its value. It means that the rotational regime of a molecule is undergoing occasional changes. For example, a probe may be undergoing slow

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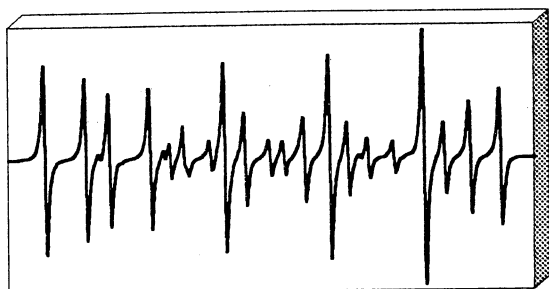
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rotation near a surface but fast rotation far from the surface. As for spin labels and probes in a sample, this leads to exchange between the two populations differing in mobility. As for rotational regimes, both may be anisotropic (in Brownian, jump, or free diffusion model). Also, g - and A -tensor values may be different in accordance to the polarity of environments.

This program is useful for extensive applications. The general model developed allows us to consider various heterogeneous systems as studied by spin-labels or spin-probes: lipid-protein membranes, polymer mixture, polymer chains grafted on a solid surface, and systems falling under the category of "interface chemistry". Also, this program may be used for taking into account the intramolecular motion, which may be classified as trans-gouche isomerization. It is also useful for spectral interpretation for some spin-labeled macromolecules. In the absence of exchange, the program works like Freed's for nitroxides undergoing anisotropic rotations. No doubt any value of magnetic resonance field is possible in the computations. Computation is rapid; it takes no more than 5 minutes to simulate one spectrum on a capable IBM PC 486.

From Michael J. Mombourquette in John A. Weil's group, University of Saskatchewan in Saskatoon, Canada: Our Program EPR-NMR



The latest version (6.01) of our program EPR-NMR, in the form of both a diskette bearing the FORTRAN source code and utilities, and also a much updated manual, is now available.

This program was written primarily to achieve generality and flexibility in handling magnetic resonance spectra of single crystals and powders, but spectra of low-viscosity liquids can easily be dealt with. The number of spins included and their values (non-negative half-integers and integers) is arbitrary, as is their assignment as either electronic or nuclear.

The program sets up spin-Hamiltonian (SH) matrices, and determines their eigenvalues (energies) using "exact" diagonalization. It is a versatile program, having many operating modes tailored to a variety of applications. These modes can be grouped into four *categories*, in increasing order of complexity as follows:

1. Energy-level calculation; 2. Spectrum simulation;

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3. Comparison with observed data; 4. Parameter optimization.

For each *category*, most of the operations of the lower *categories* remain available, so that a good way to learn how to use the program effectively is to start at the lowest *category* and work one's way up.

Category 1: the user provides the program with SH parameters, and directions and magnitudes of applied magnetic fields.

Category 2: the user also specifies an experiment, chosen from field-swept or frequency-swept electron paramagnetic resonance (EPR) or nuclear magnetic resonance (NMR), electron nucleus double resonance (ENDOR), or electron spin echo envelope modulation (ESEEM) line positions. Also, the user must identify the transitions of interest. The "spectra" simulated consist of sets of transition frequencies or magnetic field magnitudes, and possibly relative transition probabilities. The program can also convolute these data with a line-shape function (Lorentzian or Gaussian) to produce a plot.

Category 3: the user also supplies appropriate observed single-crystal data, with transition labels assigned, and the program determines the degree of consistency with data calculated from the given SH parameters. This can include an error analysis on a user-selected subset of SH parameters and/or magnetic-field directions.

Category 4: the user-selected subset of parameters may be optimized, so as to give better agreement between observed and calculated transition frequencies. This uses a non-linear least-squares routine which systematically varies the parameters so as to minimize weighted differences between observed and calculated transition frequencies (or fields). In this *category*, user-supplied SH parameters need only be estimates or outright guesses.

The new version of the program contains many corrections and improvements, including: Capability for NMR as well as EPR calculations; Bug fixed in ENDOR powder simulation and plotting; Multiple units now allowed with greater flexibility in their use; Diagonalization routines updated using latest version of EISPACK (with a bug fix); Automatic assignment of transition labels; Capability to handle several unpaired electronic spins; Availability of Boltzmann factors

(but not relaxation effects); New examples; Revised and reorganized manual; and much more.

We have plans for numerous further improvements, which will be installed as our time and resources permit. Our first aim must remain the continuation of our own research efforts. We will appreciate receiving word from you regarding your usage of the program, especially, any and all flaws you discover in version 6.01 and its manual, as well as suggestions for improvements that could be incorporated in the future. We intend to continue to be helpful if you contact us with questions. We would also be very pleased to receive any financial contributions to recover the considerable cost of producing and sending the program.

The program runs on any computer capable of running 32-bit FORTRAN 77. We currently have it running on several machines (operating systems): Bruker's ESP300E spectrometer computer (OS9); IBM thinkpad 700, *i.e.*, 486SX with co-processor (windows); INTEL 486DX and 386DX with co-processor (OS/2); DEC VAX (VMS); DEC alpha (VMS); HP9000 (UNIX); and on several other computers at other facilities.

Input consists of an ASCII file containing commands and data. Output can be in ASCII or in binary (for spectral output). Several types of spectral simulation files can be produced for use with any spread-sheet graphics application which can read in column formatted ASCII data (space or tab separated). It also produces output specifically formatted for the TELL-A-GRAPH package running under VMS and, as well, it produces binary files which WIN-EPR (from BRUKER) can read. The WIN-EPR option currently works properly only under OS/2, DOS, OS9 and VMS. Some UNIX machines can also produce the proper WIN-EPR binaries but this is not guaranteed.

We can supply you with a distribution diskette containing the source code and example files as well as some utility files installing it on the machines we can access here. There is also a printed manual, complete with theoretical discussions and examples of options available in the program, as well as descriptions of all the sample files on the distribution diskette, including the graphic output as applicable.

To use this program on a PC, you will need at least a 386 with a math co-processor and 8 MB RAM minimum. I

suggest at least a 486 DX/33 with 12-16 MB RAM running under OS/2 using Micro-Way's NDP FORTRAN for OS/2. It is far faster and more efficient than an equivalent DOS/Windows system. I use this software combination on a 486 DX2/66 with 16 MB RAM running OS/2 2.11 on a day-to-day basis as my development platform.

We do not formally sell the program but do make it available (there are ca. 80 users at this point). We are a financially stressed group here and our EPR-NMR project has been surviving on the donations of groups who use our program. The average donation for the program is US\$400 but any amount you feel affordable (some users have given as much as US\$6500 and others have given as little as US\$50) is acceptable. Please consider at least covering our printing and shipping and handling costs. Contact Dr. John A. Weil or Dr. Michael J. Mombourquette at the Department of Chemistry, University of Saskatchewan, 110 Science Place, Saskatoon, SK S7N 5C9, Canada.

From Yang C. Fann, Northwestern University in Evanston, Illinois.

Listed below are URLs of EPR web sites I have collected and checked out since January '95. If anyone finds or has any new (updated) info on this list, please feel free to contact me. (Editor's note - please also let us know as well so we can publish updated lists of URL's and web pages).

- <http://ierc.scs.uiuc.edu> — at the Illinois EPR Research Center (IERC), Urbana
- <http://alfred.niehs.nih.gov/LMB/home.html> — at the Laboratory of Molecular Biophysics at NIEHS
- <http://emrs.chm.bris.ac.uk> — at the EMR WWW Server at Bristol, UK
- http://www.biomed.abdn.ac.uk/ftp/home/pub/esr/epr_db.html at Dr. Richard Partridge's WWW EPR Database Server, UK
- <http://dirac.chem.jyu.fi> — the EPR Server at the University of Jyvaskyla, Finland
- <http://141.106.72.102/BRI-EPR> — at the National Biomedical EPR Center at Milwaukee
- <http://chm15127.usask.ca> — the EPR Group (Dr. John A. Weil) at Univ. of Saskatchewan, Canada
- http://amethyst.cbs.ogi.edu/JSB/XOP_page.html — Dr. John Boswell's EPR Simulation program (Igor Pro)

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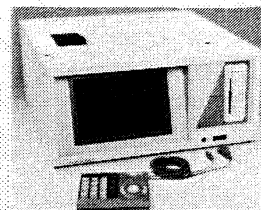
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- <ftp://xenon.che.ilstu.edu> — Xenon: EPR-list FTP Server at Illinois State University

You may find links to these servers from many of the others, including our Webserver at

- <http://endor1.chem.nwu.edu/epweb.htm>
Have fun browsing!!

EPR SPECIALIST VIGNETTES

Edited by
Arthur Schweiger

HIGH-PRESSURE EPR

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1. Introduction

High hydrostatic pressure is an important variable, complementary to the temperature in investigations of a wide variety of properties of condensed phases. Different

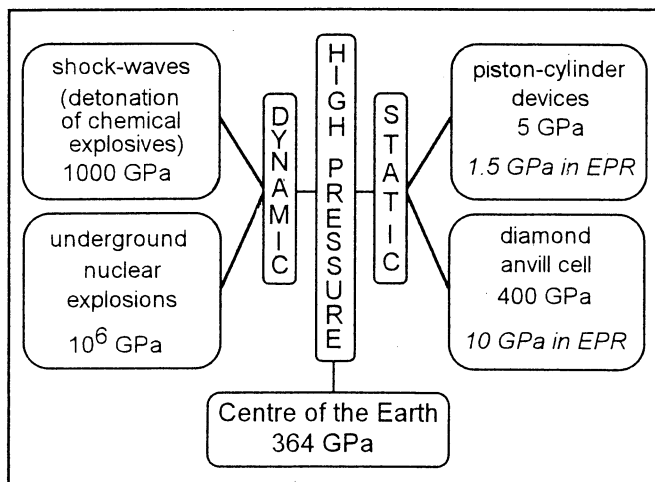


Figure 1: High-pressure techniques (1 bar = 0.1 MPa = 14.5 psi = 0.986 atm).

techniques are used for generating high pressures (Figure 1). In EPR spectroscopy only static techniques are used. The piston-cylinder devices were introduced to EPR by Walsh and Blombergen¹, and currently the safely achievable pressure is of about 1.5 GPa. Higher pressures, up to about 10 GPa, can be obtained in EPR resonators by use of

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compact diamond anvil cells, as first designed by Sakai and Pifer², with pressure gasket acting as a X-band microwave resonator. This technique is restricted in many applications by the very small volume of the resonator available for a sample (10^{-2} mm^3) and by unsatisfactory parameters of the microwave resonating circuit. Moreover, a rather small gain in pressure can be obtained with diamond anvil cells as compared to the piston-cylinder technique; thus, this latter method is commonly used in EPR spectroscopy with various designs of the resonance cavities. We have used this technique for over twenty years³⁻⁵, and the recent applications in studies of weakly exchange-coupled paramagnetic crystals are reviewed together with description of high pressure techniques.⁶ Below we will review briefly the high pressure systems currently used in EPR experiments and then we will describe a few EPR results from samples under high pressure to demonstrate prospects of this method in investigations of solids.

2. Piston-Cylinder High Pressure Systems

Pressures up to 300 MPa can easily be attained with a manual hydraulic pump without a pressure intensifier. The pressure is obtained through mechanical compression of a hydraulic liquid or an inert gas. Various liquids can be used as pressure transmitting media such as light oil (as paraffin oil), benzol, petroleum ether, n-heptane, 2-methylbutane, 1:1 mixture of n-heptane and isopentane, methanol-ethanol mixture (1:1), which have freezing temperature sufficiently high under pressure and have low dielectric losses. Most tractable liquids freeze, however, above 3–4 GPa at room temperature, and solidification of the pressure-transmitting fluid leads to the non-hydrostatic stress of an EPR sample. Thus, in high-pressure low-temperature experiments, an inert gas (mostly helium) has to be used to pressurize the system. This requires more severe safety precautions than those required when one is working with compressed liquids. Helium solidifies at 10 K under pressure 58 MPa. But because of its relatively high compressibility in the solid state, the solid helium can still transmit hydrostatic pressure if a slow cooling and temperature-cycling procedure is used.

The most commonly used hydrostatic pressure sensor is the Manganin coil gauge, which has a linear electric resistance variation under pressure up to 1.5 GPa with pressure coefficient $d \log R / dp = 2.3 \times 10^{-5} \text{ MPa}^{-1}$. A four-times higher pressure coefficient is offered by an n-type single crystal of GaAs ($n=10^{15} \text{ cm}^{-3}$) which, moreover, can measure an appreciable non-hydrostatic pressure.⁷ Higher pressure calibration and measurements can be done by the ruby fluorescence method.⁸ The pressure dependence of the R_1 ruby fluorescence line (694.2 nm) is linear to at least 20 GPa with $d\lambda/dp = 3.65 \times 10^{-3} \text{ MPa}^{-1}$.

The pressurizing system delivers the pressure-transmitting medium to an EPR resonator via a beryllium bronze capillary. The medium surrounds the EPR sample, producing hydrostatic pressure. Several high-pressure resonators have been designed for EPR microwave spectroscopy as referred to by Sakai and Pifer.² A review of various different designs of diamond anvil cell has been published by Jayaraman.⁹

In the piston-cylinder technique, a few basic designs have been proposed as we review in our recent paper.⁶ The low-Q-factor coaxial resonator is suitable for samples with strong EPR signals, whereas corundum resonators are convenient for low-temperature experiments and have relatively high Q-factor. Lockout block cavities can be used for large samples, whereas locked glass cells were designed

for chemical applications with standard EPR cavities. We have found that the most suitable for the most applications in EPR is a corundum resonator that is small enough to be placed inside the high pressure chamber and a low temperature cryostat. We use the TE_{112} -type cylindrical resonator with diameter 11 mm and length 12 mm with a quality factor $Q=2500$ and a sample hole diameter of 3 mm drilled in the center perpendicularly to the cylinder axis.

Two types of couplings between microwave waveguide and resonator are used. For temperatures higher than 100 K, a direct coupling between resonator and a standard waveguide with the matching corundum wedge can be used. This is shown in Figure 2, where our pressure system with

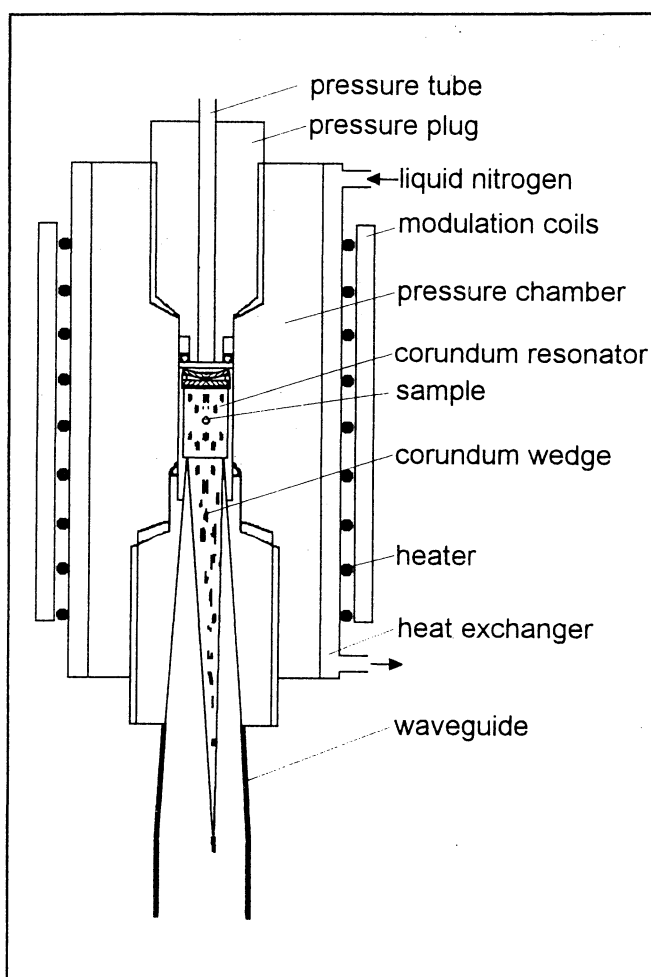


Figure 2: High-pressure system with corundum TE_{112} -resonator and petroleum ether as the pressure-transmitting medium. 100–400 K, up to 1.5 GPa, 9.4 GHz.

petroleum ether is presented. This system was successfully used for many studies in the temperature range 100–400 K under pressures up to 1.5 GPa. The high-pressure chamber with the resonating circuit can be placed in an electromagnet of 60 mm gap.

OXFORD INSTRUMENTS

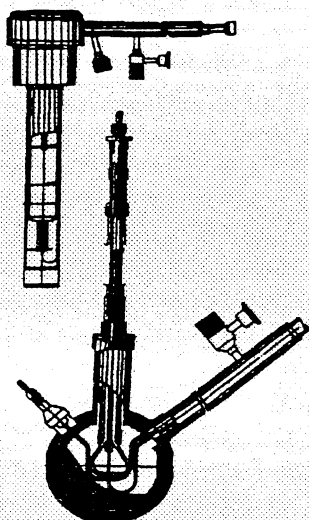
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More convenient is a coupling between the resonator and microwave coaxial line via a coupling loop. The coaxial line is coupled by antenna to the standard rectangular waveguide. Such a system, which we used for studies in the temperature range 8–400 K under pressures up to 800 MPa, is presented

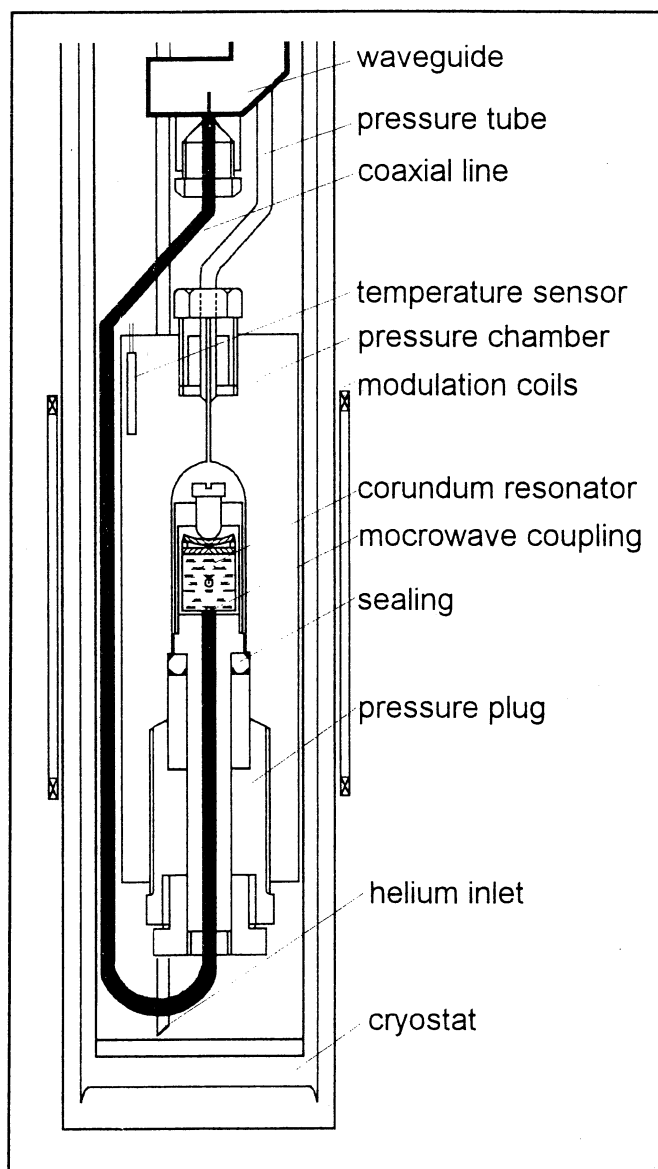


Figure 3: High-pressure gaseous helium system with TE_{112} corundum resonator in a flow helium cryostat. 8–400 K, up to 800 MPa, 9.4 GHz.

in Figure 3. The high pressure is transmitted by gaseous helium from compressor to the resonator via a flexible capillary tube. The pressure chamber is suspended in a flowing helium cryostat; gas flow is induced by a suction pump.

In both systems, magnetic field modulation of 80 Hz is provided by modulation coils mounted outside the pressure chamber or outside the cryostat.

3. Applications of High Hydrostatic Pressure in EPR Investigations

Although pressure has not found as much utility as temperature, mainly because of its experimental difficulty and some degree of danger, it is a fundamental physical variable that can affect various thermodynamic and kinetic phenomena. Any phenomenon involving volume changes will have a pressure-dependent equilibrium state, since the volume is the first derivative of the free energy versus pressure. Also, any physical or chemical process having finite activation volume will exhibit a pressure-dependent rate.

The compression (reduced volume) of a solid is the most obvious external manifestation of a decrease in interatomic or intermolecular distances accompanied by an increase in an overlap of the outer electronic orbitals and sometimes by a rearrangement of the crystal building units. Decrease in volume alters the balance of the intermolecular forces, and a new equilibrium state is adopted under pressure. It can affect to some extent many physical properties of a system. When the balance of the forces defining a system is delicate, a phase transition can appear or a new electronic ground state can be forced. However, no significant changes can be expected in the electronic structure, intramolecular structure, or molecular and lattice vibrations up to about 2 GPa, i.e. in the range of typical EPR experiments. Nevertheless, pressures below 2 GPa can stimulate phase transitions in molecular or hydrogen bonded crystals, can change intermolecular interactions, and can modify molecular motions by influence on the potential barriers. Applying high pressure allows one to separate the geometrical contributions (volume effect) from the lattice vibration contribution (thermal effect) in temperature-driven variations of a physical parameter of a system.

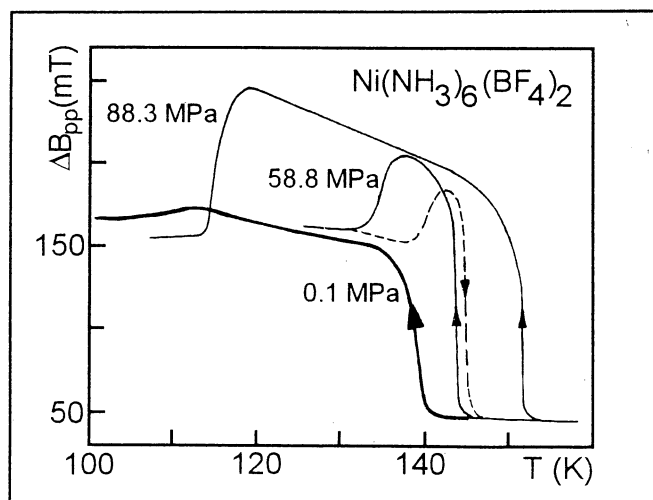


Figure 4: Temperature and pressure variations of the peak-to-peak line-width of polycrystalline $Ni(NH_3)_6(ClO_4)_2$.

Phase Transitions and Critical Phenomena

When a phase transition produces measurable changes in an EPR spectrum then it is possible to determine the temperature–pressure phase diagram of a solid. In nickel hexamines, an appreciable change in the EPR line-width appears when passing from the high-temperature cubic phase to the low temperature phase^{5,10}, as is shown in Figure 4. The phase diagram resulting from EPR measurements for this compound is shown in Figure 5.

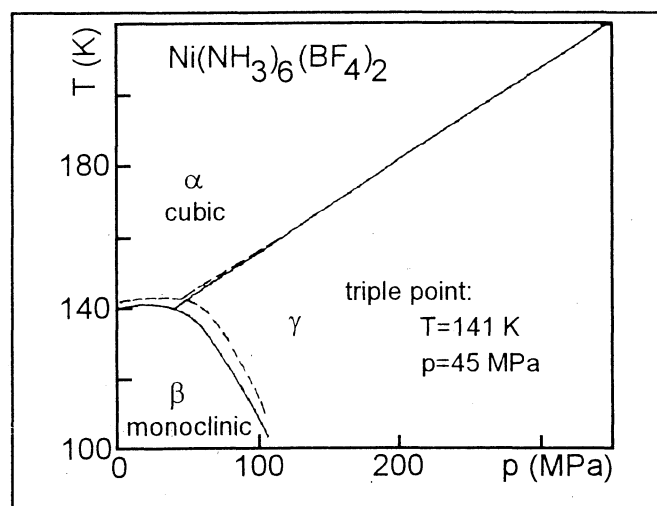


Figure 5: Phase diagram of $\text{Ni}(\text{NH}_3)_6(\text{ClO}_4)_2$. Dashed lines indicates temperature hysteresis (see Figure 4).

EPR investigations under hydrostatic pressure allow one to study the critical phenomena in the vicinity of a phase transition. Results for the $\text{Gd}^{3+}-\text{O}^{2-}$ complex in RbCaF_3 ¹¹ are shown in Figure 6. The cubic-to-tetragonal phase transition temperature ($T_C=194$ K) is shifted to higher temperatures under pressure with simultaneous increase in the discontinuity of the order parameter ϕ at T_C . The cubic spin-Hamiltonian parameter b_0^4 of Gd^{3+} increases under pressure, whereas the critical exponent, defined in $\phi=A(T-T_C)^\beta$, is reduced from 0.28 to 0.23 at 800 MPa.

Effect of Pressure on the Spin-Hamiltonian Parameters

The zero-field splitting parameter D of multielectron paramagnetic ions is influenced by temperature and pressure, and as a rule an increase in pressure acts like a decrease in

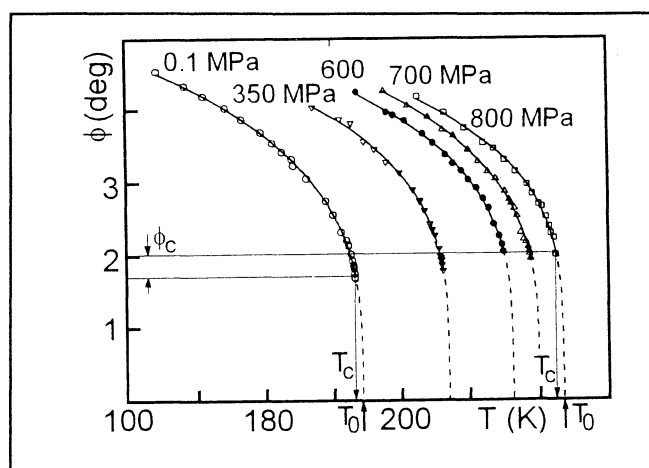


Figure 6: Temperature and pressure variations of the order-parameter ϕ in cubic-to-tetragonal phase transition in $\text{RbCaF}_3:\text{Gd}^{3+}-\text{O}^{2-}$.

temperature. The temperature dependence of D , i.e. $(\partial D/\partial T)_p$ is governed by two contributions: from changes in the geometry of the paramagnetic complex caused by thermal lattice contraction and from lattice vibration due to the spin-phonon interactions. EPR studies under pressure allow one to separate these two contributions. For cubic symmetry, these contributions are related by simple thermodynamic equation

$$(\partial D/\partial T)_p = (\partial D/\partial T)_V + (\alpha_V/\beta_V)(\partial D/\partial p)_T,$$

where α_V and β_V are volume thermal expansion and compressibility coefficients, respectively. (Typically $\alpha_V/\beta_V=-3$.) The measurements of $\alpha\text{-LiIO}_3:\text{Cr}^{3+}$ have shown that the phonon contribution to the $D(T)$ is very small and does not exceed 2%.¹²

A similar separation procedure can be applied to other spin-Hamiltonian parameters. The fine structure parameter b_0^4 of Gd^{3+} and Eu^{2+} in CdF_2 measured under high pressure allowed one to deduce that 70% of the temperature induced changes in b_0^4 are due to the thermal lattice contraction.¹³

Pressure Tuning of the Weak Exchange Coupling

Temperature and pressure variations of a weak exchange interaction have been reported in many copper(II) compounds.⁶ Both increase and decrease in exchange integral J was observed. In $(1\text{-phenyl-3,5-dimethylpyrazole})_2\text{CuCl}_2$ with square-planar CuN_2Cl_2 coordination, the exchange

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coupling is very weak, with $|J|=0.00386(5) \text{ cm}^{-1}$ at 292 K, and is temperature-independent. However, the J -value decreases under pressure and, moreover, becomes temperature-dependent under pressure (Figure 7).¹⁴ This behaviour was explained as a result of a bending of the pyrazole ring by high pressure and a shortening of the Cu-N bonds due to an anisotropic compressibility of the crystal.

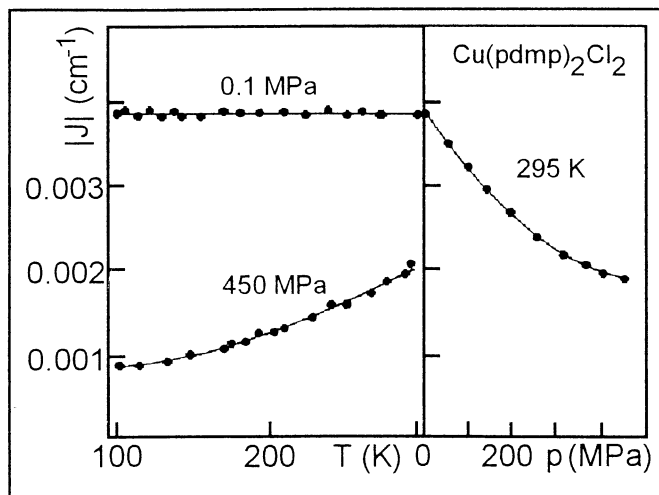


Figure 7: Temperature and pressure dependence of the exchange integral J in (1-phenyl-3,5-dimethylpyrazole)₂CuCl₂ crystal.

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BUILDING THE PERFECT BEAST

Chris Bender
NIH Biotechnology Resource for Pulsed EPR

MORE NOTES ON THE SET-UP AND OPERATION OF ENDOR COILS

I need to begin this installment with a clarification of some points on the Ruthroff impedance matching transformers that I previously described.¹ First, their ideal 'match', that is 1:4, etc., applies to a constant impedance Z . In other words, if you have a resistive load of 12.5 Ω , then you will observe a fairly flat response over a bandwidth that is determined by the transformer. On the other hand, if your load is reactive, for example, a coil or capacitor whose impedance is frequency dependent, then the transformer is not going to compensate for that change in Z , and you will still observe power fluctuations as you sweep. My operating procedure entails determining the impedance of the coil/cavity assembly at the center of my sweep frequency, then building a transformer to match that impedance to 50 Ω . I then sweep only a 10 MHz range at a time ($f_C \pm 5 \text{ MHz}$).

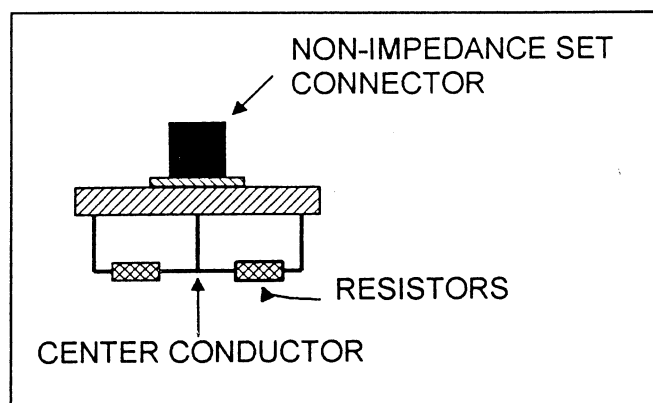


Figure 1: Construction of resistive loads 'standards' for radiofrequency design. Six or more resistors are connected in parallel between the connector's center conductor and ground (casing). The load should be encased in a metal can.

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If you intend to build coils, I suggest that you make yourself some 'standard' loads to aid in preparing the transformers. I use 6 or more carbon composition resistors ($\frac{1}{2}W$) arranged in parallel as a low power resistive load, and I build the load as symmetrically as possible in a can with a

non-impedance rated UHF or TNC connector (Figure 1). The same construction technique can be used to fabricate a reactive load by installing a network (combinations of inductors and/or capacitors) instead of simple resistors. Although these are useful and necessary test components, I tend to rough design with a 50 Ω BNC bulkhead fitting (Figure 3) that cuts down on the amount of soldering I have to do.³

In the previous note¹ on transformers I mentioned that I had not verified that a non-impedance rated connector behaved differently than one rated at 50 Ω, although I have used non-impedance rated connectors on the non-50 Ω side of my transformers and on circuit interfaces. Figure 4 illustrates the result of a test. I set up two directional couplers in an opposing manner so that one sampled the transmitted rf power, and the other sampled the reflected power. The 'coupled' port is fed directly to my oscilloscope inputs A & B. You may recognize this as a low-tech VSWR meter.

Put one directional coupler in the circuit so it will sample the rf power going from source to load, and the second so the coupler will sample the rf power reflected back to the source.⁴ On the Minicircuits ZDC-20-3, the ports are IN, OUT, CPL, and therefore the cables should be connected source to IN-1, OUT-1 to OUT-2, IN-2 to the device under test. Both CPL ports go to the scope. Figure 4A-C illustrates resultant oscilloscope traces for a 50Ω load, open circuit, and short circuit.

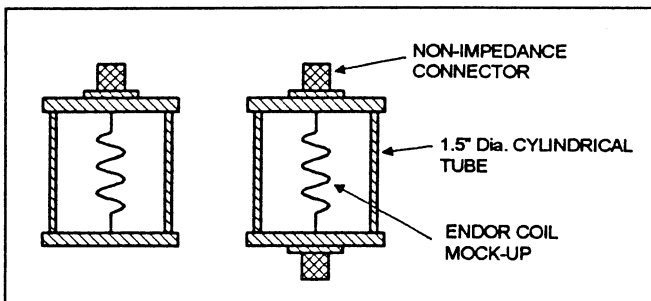


Figure 2: Inductive loads for prototyping impedance matching networks for a TM_{110} ENDOR cavity. The 1.5" dia x 4.0 cm length cylinder roughly matches the dimensions of a 9.5 GHz resonator. Cavity on left is an inductive shunt; on right is an in-line unit that may have network elements put on either end.

The traces designated 4A are what you observe with the source (rated at 50 Ω) fed to a standard 50 Ω load; the transmitted power is fully 'absorbed' by the load. This is what is supposed to happen on a transmitter (and ideally, your ENDOR). The next pair of traces (4B) was obtained with an open circuit (no termination of the cable); transmitted and reflected power are about equal. Traces 4C is a 50 Ω cable terminated with 12.5 Ω resistive load. Trace 4D is the same 12.5 Ω load matched with a 1:4 Ruthroff transformer with 50 Ω BNC connectors as the interface between the transformer and load. Trace 4E is the same load matched with the same transformer, but there is no impedance rated connector between the two elements (direct solder, or a non-impedance rated UHF or TNC connector).

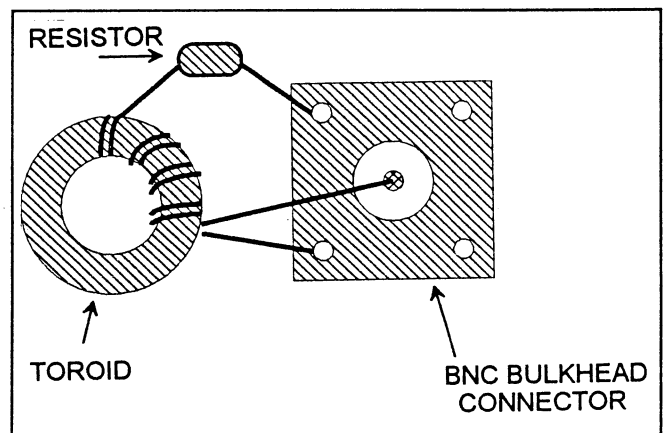


Figure 3: Quick method of testing matching properties of a toroid transformer. A panel jack BNC connector is used as the 50 Ω interface to the transmission line. A resistive 'load' is attached between the toroid and the BNC panel outer shield; the toroid ground lead is similarly attached; leaving only the high impedance side of the toroid to be soldered. Useful for rapidly determining the optimum permeability and physical dimensions of a transformer when used with opposing directional couplers.

Assuming that the transformer is suitably designed, the next task to tune up a coil. An inductor will have a linear Z vs. frequency profile up until it goes into resonance. For the 10 mm coils that you ordinarily stick into a Bruker cavity, the resonant frequency is well over 100 MHz, but you will get resonances at lower frequency because of parasitic

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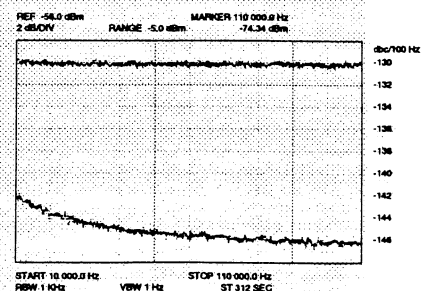
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capacitance to the cavity wall (the whole cavity assembly is a reactive network). Most of my 20 or so turn coils have a 15 MHz Z of about 12Ω , so I'm all set to go with a simple 1:4 transformer. At higher frequencies Z may be higher, or I may encounter an unwanted resonance.² If the impedance is too high, I can use a transformer with a different ratio, or I can stick in another reactive element to bring the total network Z back down to some manageable value. When I have a spurious resonance, I put in another reactive element to eliminate the resonance and then match for the new Z (the spurious resonance problem is covered in ref. 2).

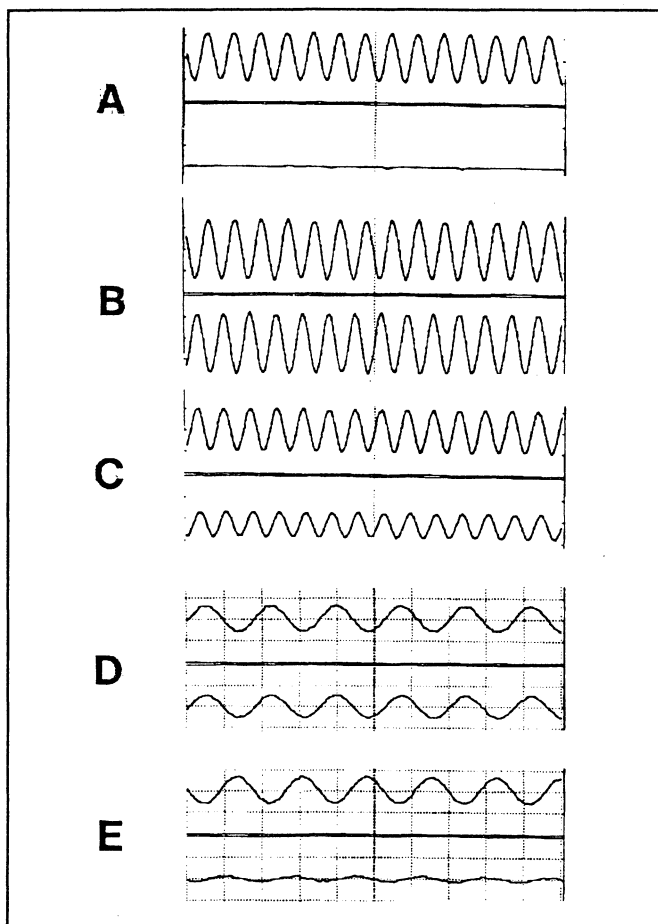


Figure 4: Transmitted (top) and reflected (bottom) waveforms passed through a transmission line terminated with A: 50Ω load, B: open circuit, C: 12.5Ω load, D: as (C), but with 1:4 Ruthroff transformer, 50Ω connectors each end of transformer, E: as (D), but without 50Ω connector on low impedance side of transformer.

In brief, one can rationalize coil design from our experience with the microwave cavity. Think about your typical cw-EPR cavity - narrow 'dip', high Q , miserable bandwidth. Pulsed EPR cavity/resonator - broad 'dip', lower Q , less miserable bandwidth. The dip on the oscilloscope is power vs. frequency through a bandpass filter (your cavity). As the Q drops, the dip flattens and the bandwidth increases.

For an EPR experiment at fixed frequency, you want a high Q , narrow bandwidth.

The ENDOR coil is a low frequency filter structure identical in behavior to the microwave cavity (in fact, for a limited number of bands one can make helical microwave resonators). The same argument as above holds, except that, because you are sweeping the frequency, you want a high bandwidth, low Q . The design task, therefore, is to make a coil that features a low Q , high bandwidth while maximizing the field (usually equated with high inductance in a solenoid). These are not mutually compatible design parameters, and you can pencil and paper trade-offs using standard formulae.⁵

PULSED ENDOR - The matching strategy that I use for cw-ENDOR can be adopted for used in pulsed ENDOR, although I find that I have to worry a little bit about the coil Q . If the coil rings (a function of Q), the ringing may put a significant rf field in my (Mims) cavity at times when I may deliver a microwave pulse. My electrical rf impulse may be well within the temporal spacing between the microwave pulses, yet a long ringdown may leave me with a significant rf field long (several microseconds) after the rf impulse is applied; any rf field that lingers into the microwave pulse application time will wreck havoc on the spin dynamics of the electron, giving you a spurious suppression of the echo intensity and a false 'ENDOR line'.

A related problem with ESE-ENDOR is transmitter noise that puts a small, but significant rf current through the coil even though you may not be driving the transmitter with an 'ON' pulse. In the previous note, I described the use of a pulse transformer with the amplifier's blanking switch to rectify this problem.¹ I have since dispensed with this solution in favor of crossed diode switches, which are the method of choice for NMR spectroscopists.

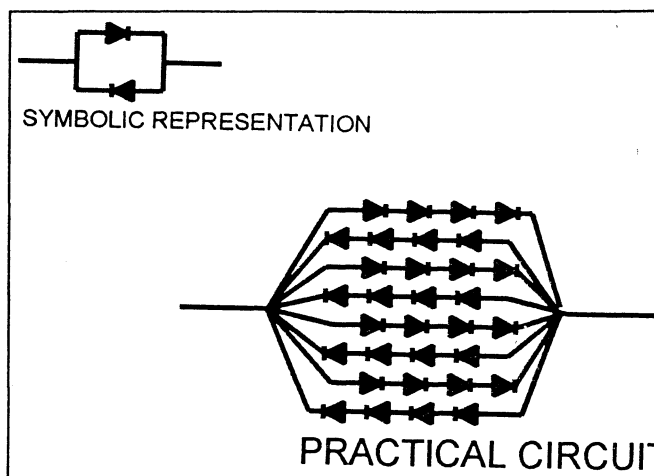


Figure 5: Signal diode switch used to eliminate transmitter noise from ENDOR coil. A practical switch will consist of four crossed pairs, each consisting of up to four diodes soldered together in series (see text for details and rationale).

As it turns out, NMR spectroscopists have a similar problem: their receivers must be able to detect small signals uncorrupted by the same rf amplifier leakage that plagues the pulsed ENDOR experiment. A good starting point for anyone, therefore, is the Fukushima/Roeder book on NMR instrumentation.⁶

The first modification that I made to our ENDOR unit was to decouple the timing of the low power GaAs FET switch and the blanker pulses. I had been using a Datapulse generator that delivers positive and negative (complement) pulses, which was convenient for simultaneously driving the rf modulator and the amplifier. With such an arrangement, however, I was stuck with a poor leading edge on the rf pulse (see the figures in previous article¹) because of the slow fall of the amp's inductive switch. Decoupling the two driver pulses (analogous to what we do with the TWTA and low power pulses of the microwave circuit) allows me to turn on the rf amp and offset the input of the low power rf pulse in order to keep it square. At this point I still have some low power amp noise in the dead zone between full blanker 'off' and the leading edge of the rf pulse.

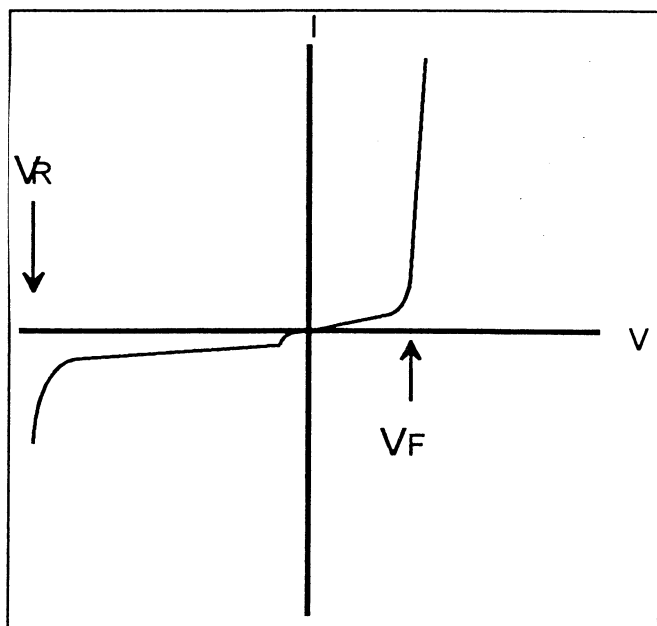


Figure 6: Current-voltage plot of a diode. A signal across a diode of amplitude less than V_F does not pass. In general, $V_F < 1\text{ V}$; V_R (reverse, breakdown) $\sim 75\text{ V}$.

Further modification of the circuit will get rid of this dead zone noise and, in principle, allow you to forego the amp's blanker altogether. The most common element for this purpose is the crossed signal diode. Silicon diodes act as switches; they conduct only when the bias voltage exceeds a threshold value. For example, a 1N914 signal diode⁷ features a V_F of 0.7V, and therefore noise of about 0.7V or less will be blocked. If your noise is greater than 0.7 V, you must add additional diodes in series until the sum of their V 's

exceeds the anticipated noise level. The problem that you will encounter, however, is that the noise level will scale with the gain setting on the amp, so I advise that you build modular circuits.

My basic diode switch unit consists of four diodes in series and, because of the relatively large currents that will pass when the pulse is applied, I assemble the four-diode series as four antiparallel pairs (a total of 32 diodes). The diode arrays are arranged on a conventional phenolic perfboard. I put the different directions on opposing sides and space each series by one column on the board; the finished board is wrapped in glass electrical cloth before being put into a Pomona box (the tape acts as insulation from the box's walls - glass cloth because this thing will get hot).

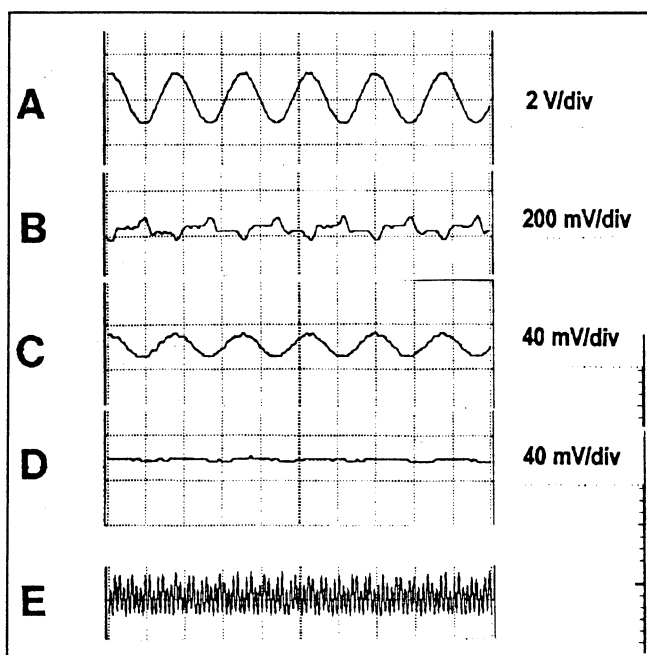


Figure 7: Oscilloscope traces of an rf signal passed through two types of diode 'switches'. A: unimpeded signal. B: Signal passing four parallel arrays (crossed) of four 1N4148 diodes in series. C: Signal passing a single 1N4148 diode (crossed pair) abutted with a reverse direction Zener diode. D: same arrangement as C, front end of 200W amp, with a lowpass filter. E: same as D, no filter. Traces A-C use a PTS 160 synthesized source as input.

Figure 7 illustrates the results of passing an rf signal through crossed diode arrays. Figure 7A is the magnitude of the signal from a PTS synthesizer that just begins to be detected when the diodes are installed. The trace illustrated in 7B is the signal that leaks through four series diodes at that threshold level. It is possible to obviate serial diode arrays by using a backward-oriented Zener diode in combination with a single silicon diode, and figure 7C illustrates leakage through a single pair of Zener/silicon diodes. What makes an immediate impression (on me, anyway) is that the Zener/silicon combination gives me comparable suppression of low power signal plus less

distortion of the signal that comes through at the threshold level (for what it's worth). It also seems to work much better on the amplifier output.

I should also point out that high-frequency amplifier noise makes it necessary to put a Minicircuits low-pass filter (DC-70 MHz or 100 MHz) on the amplifier output. Such an arrangement gives me a very clean transmitter output when the amplifier is fully powered up and the modulator switch is closed (compare Figures 7D & E).

The diode arrays work reasonably well as a stand-alone unit and you can add boxes to meet the noise levels of different gain levels. The amplifier also has a blanker that can be used in combination with the diodes.

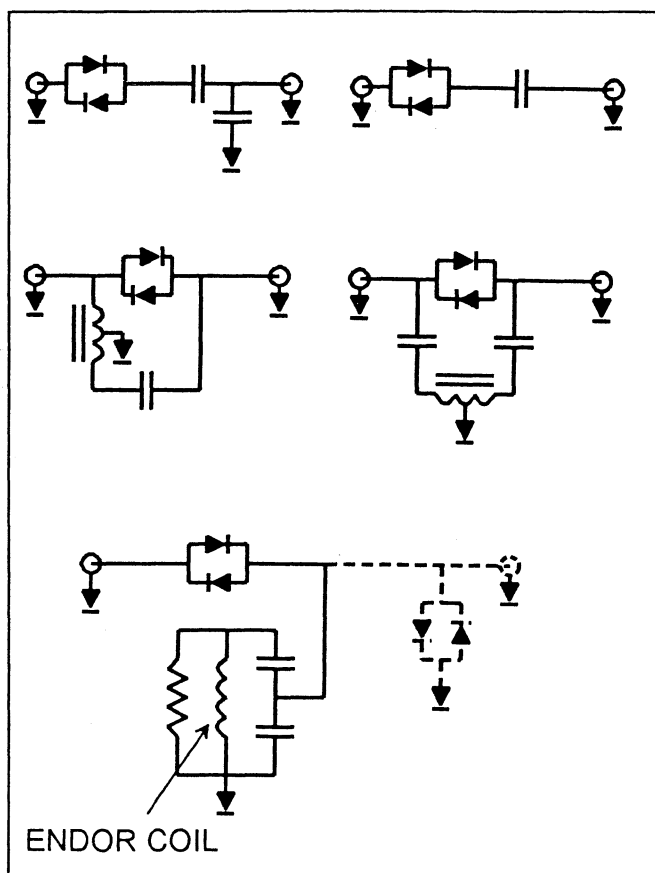


Figure 8: Transmitter Circuits for Pulsed ENDOR. All are built as boxes that go between the amplifier output (leftmost connector, as depicted) and coil. The bottom circuit is a complete system based on Edmond's NQR spectrometer - dashed lines are added elements for an NMR.

The blanker gives me an additional 30 dB noise attenuation and keeps the diodes from overheating when I have the gain high, but it still has an inductive 'kick' (again, see the previous article) that I want to tame. I made a catalog of NMR transmitter circuits and built several, which are illustrated in Figure 8. They all work well both with and without the amp's blanker. The bottom circuit is an adaptation of Edmond's NQR spectrometer, and I have been

experimenting with the Mims ENDOR cavity and Edmond's transmitter circuit (add a receiver) as a means to perform solid state NMR and NQR spectroscopy.⁸ My favorite transmitter circuit is transformer based and better suited to the swept frequency pulsed ENDOR experiment because it is inherently more broadband. It is therefore better suited to broad sweeps (by broad, I mean tens of MHz).



DISCLAIMER: At times, however, no amount of effort is rewarded, and frustration must be vented by some other means.

You have to remember when devising an ENDOR system that the circuits are not broadband. In other words, you are not going to sweep 5 - 50 MHz and expect to see a normal looking spectrum. All of these circuits behave as though they are bandpass filters. These means that you will find some optimal 'matched' frequency plus or minus some deviation over which a decent amount of power will pass (usually denoted $f \pm \Delta f$, where Δf is the point where the power at f is reduced by 3 dB - think of a cavity, Q , and the power throughput). The proper operating usage is therefore to 'tune' the matching circuit at the center of the desired sweep range, which should coincide with the operating range (the 3 dB limit) of the matching circuit. The alternative is a servo-driven tuner that constantly adjusts the matching circuit.

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2. C. Bender; G.T. Babcock, Review of Scientific Instruments, 63, 1992, 3523-4.
3. The 'load' is an appropriate carbon $\frac{1}{4}W$ resistor grounded with a 4-40 screw to the bulkhead panel mount; its other lead pigtailed to wrap around the appropriate transformer lead. The transformer ground lead is likewise attached to the bulkhead via a 4-40 screw, leaving only the transformer's 50 Ω lead to be soldered to the BNC center

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conductor. This short cut speeds up trials of toroid design when the number of turns, core permeability, and wire gauge are unknown factors.

4. Do not perform any of these tests with an amplifier; use a low power rf source only.
5. Abrie, P.L.D. The Design of Impedance-Matching Networks for Radio-Frequency and Microwave Amplifiers. Artech, Norwood 1985.
6. E. Fukushima; S.B.W. Roeder Experimental Pulse NMR: A Nuts and Bolts Approach. Addison-Wesley, Reading 1981.
7. Besides 1N914 I also use 1N4148 silicon diodes. They both run about \$0.20 apiece from Newark Electronics.
8. For those interested, it does work for very strong signals (so far). I recommend, however, that one use the NMR spin echo and swept frequency/field method of measurement, rather than an FID-based method.

Miscellaneous Note: For rapid prototyping work with integrated chips (ICs), it is often more efficient to flip the IC over, glue it to a perboard, and solder the cables directly to the prongs. The radio amateur guys call this the 'ugly' or 'dead bug' method of prototyping, for obvious reasons. For rough work, it definitely beats wire-wrapping and avoids the high cost of plated prototyping boards (some Vectorboards run about \$25 apiece). Providing you can live with the derision you will incur (invariably, people are going to think

you've failed an IQ test when they see these things mounted upside down), the only drawback is that you need to orient the ICs the same way so as to not forget which pin is which, numerically.

TIPS & TECHNIQUES

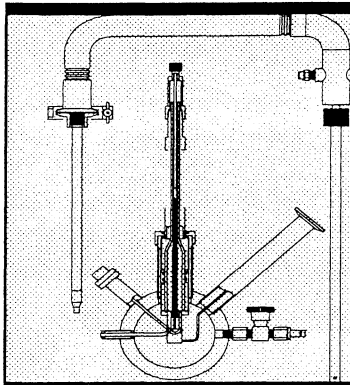
Miscellaneous Tips for EPR Users

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Research Specialties

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This month's most unusual failure of EPR equipment revolves around our old friend the Xenon/mercury vapor lamp. The leads to the lamp and starter circuit coupled enough high frequency energy into the Varian spectrometer (Bruker, JEOL and home-built spectrometers are equally prone to this type of failure) to destroy two transistors and one hybrid circuit in the 100 KHz high frequency receiver module, specifically the phase detector and driver. These high frequencies produce standing waves on the wiring inside the spectrometer, thereby producing high voltages at various unpredictable spots inside of the spectrometer. This can cause failures anywhere inside the spectrometer. The term high voltage at this point is relative, since destruction levels for solid state devices vary from just a few volts to maybe a few hundred. The worst part is that localized damage may not show up immediately and/or just may become a source of noise or instability possibly distributed throughout the system that you may live with for a long time. From a previous issue of the Newsletter are comments on this type of problem:

Xenon/mercury vapor cw-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



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for the lamp and numerous leads associated with the EPR act as antennas to transmit and receive 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 and 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.

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

NOTE: This could lead to a future product: an EMP-hardened spectrometer. Just add an extra \$100,000 to the price. Of course, we could consider a ban on all Xenon lamps that are unshielded. Another approach is to start it down the hall using an extension cord plugged into someone else's lab. After starting the lamp, it can be rolled down the hall to the spectrometer. (In a pinch, this actually works, depending on whose lab is down the hall!) Anything that disturbs the Y-axis on the recorder or oscilloscope is a sign of excessive input and should be addressed immediately.

An Observation of Artifacts in EPR Spin Trapping: Free Radicals Produced by a Polytron

Jinjie Jiang^{1†}, Ke Jian Liu¹, Li Li Ji², Harold M. Swartz^{1*}

Spin trapping techniques with EPR detection have proven to be of great value, extending capabilities to study short lived species to a variety of biological and other systems. The technique also has proven to be unexpectedly quite complex; it is sometimes observed that "someone who is new to spin trapping can produce a manuscript after a few weeks

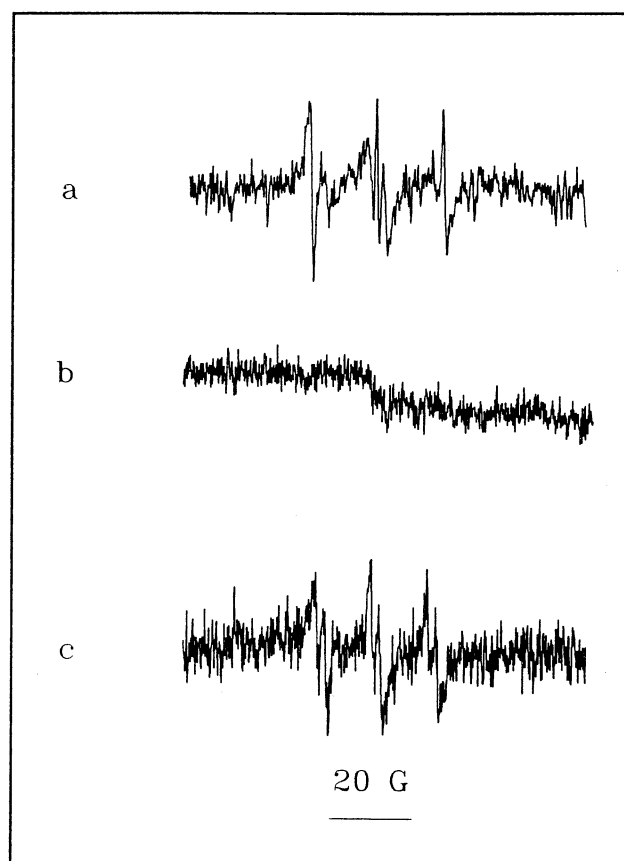


Fig 1 -- a: Spin adduct signal observed in an extract of muscle prepared with the Polytron. Fresh rat skeletal muscle (10 g) with 10 ml saline containing 15 mM PBN was homogenized with a Polytron. EPR spectrometer settings were: scan range 100 G; field center 3254 G, modulation amplitude 1 G; incident microwave power 10 mW; average of 10 scans. b: EPR spectrum from an extract of frozen-pulverized rat skeletal muscle. The instrumental settings were the same as in (a), except that the gain was 5 times higher with an average of 30 scans. No spin adduct signal was observed. The small signal in the center could be either from trace amount of the ascorbyl free radical or from the free radicals produced by pulverization¹. c: Spectrum from H₂O and chloroform mixture (1:1) with PBN (15 mM); spectrometer settings the same as in (a), with 1 scan.

of experiments, while those who have been in the field for a long time require months or years"¹! One of the principal reasons for this observation is the potential for observing "trapped species" which, in fact, have been produced through an experimental artifact. As an illustration of the general problem and to provide insights as to the potential of artifacts in a particular experimental approach which is used fairly widely, we have prepared this report.

Previous reports have indicated that various preparation methods including quick freezing¹, mechanical grinding,^{2,3} use of plastic syringes,⁴ and ultrasound treatment⁵⁻⁷ may produce free radicals. We report here the effects of a commonly used tissue homogenizer, the "Polytron".

The Polytron consists of a metal (usually stainless steel) housing and a metal shaft (blade) driven by a motor. The

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gap between the metal housing and shaft is very small. The metal shaft revolves at a rapid rate (several thousands rpm), breaking cell membranes, releasing the intracellular constituents.

A homogenate of muscle tissue in the presence of phenyl-tert-butyl nitron (PBN) was prepared using the Polytron (model PT-10, Brinkmann Co.) at 4000 rpm and the resulting homogenate was then extracted by chloroform and methanol (2:1). After the separation of the organic phase from the aqueous phase, the organic solvents were evaporated by N₂ gas, and the sample was reduced to <100 ml. A weak spin adduct signal was observed at 9.6 GHz (Fig 1a).

As a control, muscle was frozen in liquid N₂ and pulverized with aluminum tongs. The powder then was treated by the extraction procedure as described above. No spin adduct signal was observed (Fig 1b).

To determine whether the free radical that was produced by the Polytron was generated by the mechanical grinding or by ultrasound generated by the device, we studied samples containing only PBN in a mixture of water and chloroform (1:1) (chloroform was used because PBN is much more soluble in it and PBN spin adducts are unstable in aqueous solutions). The mixture was treated with the Polytron and separated. The organic phase then was reduced by blowing N₂ gas to reach a final volume of <100 ml. An EPR signal of a spin adduct was observed (Fig 1c).

Although the splitting constants of the spectra in Figure 1a and 1c are slightly different, we believe this is because of solvent effects. We conclude that the signal we observed in Polytron-treated muscle is most likely from free radicals produced by the ultrasound generated by the Polytron.

There are some reasonable ways to avoid becoming confused by artifacts such as the one described here. Perhaps the most important thing is to be aware that the presence of a spin adduct does not necessarily mean that a postulated reaction took place and the resulting radical was trapped by the spin trap. Be aware of the many different pathways that can lead to the presence of a spin adduct. In addition to this type of general awareness, careful attention should be made to include controls at various points in the experimental procedure to determine if the spin adduct can be produced without one of the principal experimental variables. It also is highly desirable to repeat the experiment with a different spin trap, preferably one that is quite different from the original spin trap that was employed, because many of the

artificial signals are quite sensitive to the type of spin trap that is used.

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FROM EPR CENTERS**Notice regarding the EPR Research Resource Centers in the USA:**

The Biotechnology Resource in Pulsed EPR Spectroscopy (Bronx, New York) has a new brochure describing its capabilities; it is available upon request from Prof. Peisach (address on front page of this Newsletter). We point out here that a convenient source of considerable information on each of the EPR Centers, including listings of recent publications, is the corresponding World Wide Web page. Prospective users and others interested in activities of these Centers are encouraged to look at their WWW network entries:

Biotechnology Resource in Pulsed EPR Spectroscopy:

<http://spin.aecom.yu.edu/>

Illinois EPR Research Center (IERC):

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

National Biomedical ESR Center:

<http://141.106.72.102/BRI-EPR/>

The Directors of the Resources welcome suggestions for improving the usefulness of their WWW pages.

For more information about EPR on the World Wide Web, see the Computer Corner in this issue.

CONFERENCE REPORTS

The L.H. Sutcliffe Celebration and Symposium on Magnetic Resonance (March 25th, 1995, University of Surrey)

(Report by Reef (Philip D. II) Morse*)

I once heard that as spectroscopists age, they become more relaxed. At the L.H. Sutcliffe Symposium on Magnetic Resonance, held March 25th, 1995 at the University of Surrey, Guildford (UK), Les was feted by his friends and collaborators for his life of accomplishments in the field of magnetic resonance, but Les himself didn't speak. Indeed, he sat back, relaxed, and enjoyed the event.

The gala tribute to Les, organized by Jim Emsley, Jim Feeney, and Duncan Gillies, and attended by more than 90 persons, began with a brief history by Peter Butterworth, the Senior Pro-Vice Chancellor of the University of Surrey, of the events leading to Les' transfer from Royal Holloway College. He emphasized the major enhancement of magnetic resonance at Surrey by Les's arrival.

The symposium itself began with an introduction by Alwyn Davies (Chairman of the ESR discussion group) followed by a talk by Martyn Symons about how EPR can tell you about the effects of ionizing radiation by identifying radicals formed which in turn identifies the chemical processes which are induced by the radiation, specifically, where electrons go initially, and what happens to them at equilibrium. Keith Preston followed with a lecture on cluster nitrosyls, showing how EPR has revealed the mode of NO bridging between ions in $\text{Fe}_4\text{S}_4(\text{NO})_4$. Keith spoke of his

collaboration with Les and Les' interest in nitrogen-sulfur heterocycles. Keith presented Les with a T-shirt proclaiming Les the "King of the dithiazolyles". John Morton next discussed his work on fullerene EPR and how the electron distributes over the carbon lattice in C60 and C70 fullerenes. He showed that EPR can distinguish between electrons in the hexagons and pentagons.

The afternoon session on NMR was introduced by John Lyndon (Chairman of the NMR discussion group). Peter Belton spoke on NMR of food materials. His interests were concerned with the state of water and sodium ions in frozen materials. Interestingly, sodium next to proteins in frozen food products behaves just like it does at room temperature. In milk, one would expect the medium to behave as concrete, but this is not the case. Belton also showed how NMR could be used to identify flavones and sugars in pear juice to determine its global origin. Next, Jim Feeney told about his work on binding of small molecules to proteins. He used NMR to show where small molecules, such as co-factors and drugs, interacted on the protein, the shape of the small molecule-protein complex, and the dynamics of the molecules and complex. He spoke primarily about his work on dehydrofolate reductase and its interaction with methotrexate. Jim Emsley continued the NMR theme with his studies of liquid crystals and how NMR could get structural information on molecular behavior, order, dynamics, phase properties, and pre-transition behavior. Neville Boden then discussed the use of magnetic resonance in studies of ion channels and how ion channels could be stabilized by the large area per molecule of dimyristoylphosphatidylcholine. He showed convincing evidence of four phospholipids per peptide in clusters of his ion channels and suggested utility of this system in work on biosensors. Duncan Gillies concluded with a whirlwind tour of his collaborative work with Les over the past ten years. He then focused on their current work on traction fluids and their behavior (rotational and internal/segmental motion) under pressure. He showed that molecular rigidity was proportional to the traction coefficient (i.e., less motion

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makes for a worse lubricant). He also discussed their work on foodstuffs and his work on 200 MHz EPR imaging.

John Jones, Chairman of the Department of Chemistry at Surrey, concluded the conference with a thank you to the organizers and wished Les good luck in his new position at the Institute of Food Research at Norwich.

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Fourth International Symposium on ESR Dosimetry and Applications

(Report by Anne Skinner*)

This meeting was held in Munich, Germany, May 15-19, 1995. Sponsors included the IAEA, the World Health Organization, the Russian Academy of Sciences and the European Commission, as well as the International EPR/ESR Society. Nearly 200 scientists from 47 nations attended. The organizers, chaired by Dr. Dieter Regulla of GSF-Munchen/Neuherberg, gave special emphasis to increasing the participation of scientists from the former Eastern European bloc. Over 50 papers were presented in the 13 oral sessions and about 100 posters in the 4 poster sessions. Plenary lectures were given by Dr. J. Pilbrow (Australia; ESR Fundamentals), Dr. K. Mehta (IAEA; IAEA Standardization Service), Dr. M. Ikeya (Japan; Radiation Effects in Organic and Inorganic Materials), Dr. R. Alcalá (Spain; Mechanisms), Dr. R. Grün (Australia; Dating Techniques), Dr. M. Desrosiers (USA; Irradiated Food), Dr. A. Romanyukha (Germany; Retrospective Dosimetry), Dr. Ya. Lebedev (USSR; Dosimetry-related Problems), and Dr. H. Stronks (Canada; A Low-cost EPR Spectrometer).

A novel feature of the meeting was a roundtable discussion on the future directions that research in dosimetric EPR might take. Chaired by Dr. Ikeya, founder of these meetings, the roundtable provided an opportunity for a frank discussion of the most significant challenges that scientists must resolve in order to increase the confidence of the broader scientific community in the reliability of EPR/ESR.

The proceedings of the conference are being edited by Dr. M. Desrosiers, Dr. D. Regulla and Dr. A. Skinner, for publication in *Applied Radiation and Isotopes* at the end of 1995 or early in 1996.

Participants agreed that the level of interest shown at this meeting justifies continuing to sponsor conferences on ESR as a dosimetric method. The location of the next session is not yet fixed, but suggestions include Russia, the Ukraine and Italy. It is hoped that by the time of publication of the proceedings, the venue will be known. Dr. Regulla and Dr. Desrosiers will form the nucleus of a standing organizing committee for future meetings.

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The organizers wish to acknowledge the financial support of DFG (Deutsche Forschungsgemeinschaft) and the International Science Foundation. They would also like to thank all those who participated, since it is their contributions that in the end determine the value of any meeting.

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BOOKS & PROCEEDINGS

THE CHEMICAL DYNAMICS AND KINETICS OF SMALL RADICALS, Vol. 6, Parts I and II. Edited by K. Liu (Academia Sinica) and A. Wagner (Argonne Nat'l. Lab).

Contents:

- Multichannel Radical Reactions (M.R. Heal & M.J. Pilling)
- The Reaction between CN and O₂: A Prototype Radical-Radical Reaction? (I.W.M. Smith)
- Fourier Transform Infrared Emission Spectroscopy as a Tool for the Study of Chemical Reactions (P.W. Seakins)
- Experimental Studies of Rotationally Inelastic State-Resolved Collisions of Small Molecular Free Radicals (P.J. Dagdigan)
- The HCO Potential Energy Surface: Probes Using Molecular Scattering and Photodissociation (D.W. Neyer & P.L. Houston)
- Radical Chemistry with Wave Packets (S.K. Gray & E.M. Goldfield)
- State-Resolved Studies of Molecular Dynamics by "Half-Collision" Techniques (P.D. Kleiber)
- Time-Resolved Studies of Cage Recombination Dynamics in Ionic Clusters (W.C. Lineberger et al.)
- Reactive Scattering of O(³P, ¹D), Cl(²P) and OH Radicals (P. Casavecchia et al.)
- Product State Distributions in Chemical Reactions: The Reaction OH + CO → H + CO₂ (K. Kudla & G.C. Schatz)
- Doppler Spectroscopy, a Powerful Tool for Studying Molecular Collision Dynamics (J.M. Mestdagh et al.)
- The Stereodynamics of Photon Initiated Bimolecular Reactions (M. Brouard & J.P. Simons)
- Orientation and Alignment of the Products of Bimolecular Reactions (A.J. Orr-Ewing & R.N. Zare)
- and other papers

Publication date: Summer, 1995. Part I, 500pp, hardcover: ISBN 981-02-2985-2, US\$112 (£77), pbk: ISBN 981-02-2983-6, US\$61 (£42). Part II, 500pp, hardcover: ISBN 981-02-2986-0, US\$112 (£77), pbk: ISBN 981-02-2984-4, US\$61 (£42). Available in the USA from: World Scientific Publishing Co., Inc., 1060 Main St., River Edge, NJ 07661, ☎: 1-201-487-9655, FAX: 1-201-487-9656, toll-free: 1-800-227-7562. Available in the UK from: World Scientific Publishing Co. Ltd., 57 Shelton St., Covent Garden, London WC2H 9HE, UK, ☎: 44-171-836-0888, FAX: 44-171-836-2020.

NITROXIDE SPIN LABELS, Reactions in Biology and Chemistry. Edited by N. Kochevinsky (Inst. Chem. Phys., Acad. Sci., Moscow) and H.M. Swartz (IERC, Illinois). Contents:

- **Introduction, General Considerations:** Use of Nitroxides as Contrast Agents for Nuclear Magnetic Resonance Imaging and Spectroscopy. EPR Imaging and *In Vivo* EPR Techniques. (Measurements of the Concentration of Oxygen. Measurement of Diffusion. Measurement of Viability. Measurement of Temperature.) Summary and Plan of the Book.
- **Terminology, Classification, and Distribution of the Nitroxides in Cells:** General Analysis and Terminology. Classification. Distribution of Nitroxides in Cells. (General Considerations. Distributions of Neutral Nitroxides. Location of Charged Nitroxides in Cells. Location of Doxyl Stearates and Related Lipophilic Nitroxides. Location of Phospholipids Labeled with Nitroxides.)
- **Chemical Reactivity of Nitroxides:** General Aspects. Stability of Pure Solutions. Electrochemical Reactions. Reduction. (Mechanisms of Chemical Reduction. Reduction of *p*-Phenylenediamine. Reduction by Metal Ions. Reduction of Nitroxides by Ascorbic Acid and Flavins.) Reoxidation of Hydroxylamines and Amines to Nitroxides. Interconversion of Hydroxylamines and Nitroxides. Reduction of Nitroxides by SH-Containing Substances. Reactions of Free Radicals with Nitroxides. Photochemical Reactions. Nitroxides as Redox Probes of Melanin. Interactions with Singlet Oxygen. Radiation-Induced Reactions. (Reduction Reactions. Oxidation Reactions. Radiosensitization by Nitroxides. Inhibition of Lipid Peroxidation.) Reactions of Superoxide with Nitroxides. Nitroxides as Catalysts of Radical Reactions. Spin Trapping. Challenges for Chemists and Biochemists.
- **Applications of Reactions of Nitroxides in Biophysics:** General Considerations. The Kinetics and Mechanism of Reduction of Nitroxides by Ascorbic Acid. Investigations of Model and Biological Membranes. (Transport of Ascorbate. The Kinetics of Reductions in Membranes. Reduction of Spin-Labeled Lipids. Dynamics of Lipids. Membrane Permeability and Transport of Nitroxides. Protein Mobility.) Nitroxide Reduction with *p*-Phenylenediamine in Suspensions of Membranes. The Use of the Kinetics of Reduction to Study Disease. Oximetry with Nitroxides.
- **Biochemical Basis of Reduction of Nitroxides in Membranes:** General Aspects of Reactions of Nitroxides in Membranes. Reduction of Nitroxides with Components of Biological Membranes. (Reactions with Sulfhydryl Groups. Reactions with Mitochondrial or Other Membranes Having Respiratory Chains. Kinetics of the Reduction of Nitroxides by the Electron Transport

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Chain. Microsomal Membranes. Nitroxide Binding to Cytochrome P-450. Reoxidation with the Respiratory Chain and Superoxide. Hydrophobicity and Biological Activity of Membrane-Active Substances.) Conclusions.

- **Metabolism and Distribution of Nitroxides in Tissues and Organs:** Homogenized Tissues. Isolated and/or Perfused Tissues. Nerves. Other Specialized Tissues.
- **Metabolism and Distribution of Nitroxides *In Vivo*:** General Considerations on Distribution and Metabolism of Nitroxides *In Vivo*. (Principles of Metabolism and Distribution of Nitroxides *In Vivo*. Assay Methods Used to Measure Levels of Nitroxides in Blood and Tissues. Blood and Tissue Levels of Nitroxides and Hydroxylamines. Single Administration. Repeated Administration.) Metabolism *In Vivo*. (Types of Reactions. Influence of Oxygen on the Reactions *In Vivo*. Roles of Intracellular and Extracellular Reduction. Metabolism in Organ Systems.) Physical Elimination of Nitroxides and Hydroxylamines. Distribution *In Vivo*. Conversions to Other Derivatives *In Vivo*.
- **Toxicity and the Use of Nitroxides as Bioactive Drugs:** General Aspects of Toxicity of Nitroxides. Data on Toxicity from *In Vitro* Systems. (Data from Model Systems. Data from Subcellular and Cellular Systems.) Toxicity in *In Vivo* Systems. (General Considerations. LD⁵⁰ and Other Measures of Lethal Effects of Nitroxides. Nonlethal Acute Effects. Chronic Effects.) Toxic Effects Involving the Non-Nitroxide Parts of the Spin Labels. (Effects due to Physical Interactions and/or Localization on the basis of Physical-Chemical Properties of the Nitroxides. Effects Due to Chemical Reactions of the Non-Nitroxide Portion of the Molecule.) Summary on Toxicity.
- **Metabolism, Toxicity, and Distribution of Spin Traps:** Introduction. Stability of Spin Traps in Cells and Tissues. (General Principles and Information on Stability of Adducts of Spin Traps. DMPO. PBN and Related Spin Traps. Other Spin Traps. Spin Traps and Erythrocytes. Conclusions on Stability of Spin Traps and Spin Adducts in Functional Biological Systems.) Stability *In Vivo*. Toxicity of Spin Traps.
- **Summary and Conclusions:** Introduction. Principles of Metabolism of Nitroxides. Potential Limitations of the Use of Nitroxides in Viable Biological Systems and Approaches to Overcome Them. (Bioreduction. Toxicity. Sensitivity.) Applications of Nitroxides in Viable Biological Systems which are Likely to be Affected by the Biological and Chemical Interactions of Nitroxides. Assessment of the Future for Nitroxides.
- **References**

Catalog no. 4204NLE, May 1995, c. 304 pp., ISBN: 0-8493-4204-X; Approx. US\$125.00/Outside USA \$150.00. Order from: CRC Press, Inc., 2000 Corporate Boulevard NW, Boca Raton, FL 33431, USA, toll-free ☎: 1-800-272-7737; toll-free FAX: 1-800-374-3401.

The first printing of the text *ELECTRON PARAMAGNETIC RESONANCE - Elementary Theory and Practical Applications* by John A. Weil, James R. Bolton and John E. Wertz, published by John Wiley & Sons, New York 1994, has virtually sold out and a reprinting is now being prepared. Reviews of this book can be found in: a) *Physics Today* 48(5), 71-2, May 1995 (H.A. Buckmaster), b) *The Analyst* 120, 4N-5N, Jan. 1995 (D. Collison), c) *Choice* 32(1), 399, Sep. 1994 (H. Giesche). The authors wish to thank all readers who reacted to their request to send in notice of flaws detected. Most of these will be repaired in the reprinted version. Happily there were not too many, and no major ones were detected. A listing of changes of any substance at all is now available from two (JAW and JRB) of the authors.

ADVANCES IN FLUID MECHANICS: Bio-fluid Mechanics, Edited by H. Power (Wessex Inst. of Technology, UK).

Biofluid mechanics is the branch of biology which applies fluid mechanics to the study of biological phenomena and the use of their concepts to understand these phenomena. The theory of fluid mechanics provides a means of describing the motion of fluids in biological processes in terms consistent with their functions. This book contains recent developments in the area of biofluid mechanics. Topics covered include:

- A Numerical Heart and Circulation Model to Simulate Hemodynamics For Rate-responsive Pacing.
- Orifice Flow in Stenotic and Regurgitant Valve Lesions.
- Folding Motifs, Kinetics, and Function in the Proximal Nephron.
- Numerical Simulation of Arterial Hemodynamics.
- Evaluation of Haemodialysis Systems Using Computer Simulation.
- Coupled Behavior of Pulmonary Circulation with Breathing Dynamics.
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- Computer Modeling of Cardiac Excitation.

Order from Computational Mechanics, Inc., 25 Bridge St., Billerica, MA 01821, USA; ☎: 1-508-667-5841; FAX: 1-508-667-7582. ISBN: 1562522108, 336 pages. Price: US\$150.00.

NOTICES OF MEETINGS

THE FOURTEENTH INTERNATIONAL CONFERENCE ON RADICAL IONS, Uppsala, Sweden, July 1-5, 1996. Note: THE FOLLOWING NEW INFORMATION HAS JUST BEEN RECEIVED:

The Radical Ions conference is a continuation of previous Gordon Conferences 1968-1992 (totally 12) and the corresponding conference held in Halifax in 1994. Following the traditions the conference will feature invited speakers and poster sessions with time for informal discussions. There will also be space for a number of short oral presentations.

The meeting will take place in the main building of Uppsala University, built in the center of Uppsala in the end of the last century. Uppsala is centrally located in Sweden, with excellent connections both by air (Arlanda airport), by train and by car.

The invited and contributed papers will be published in *Acta Chemica Scandinavica* as Minireviews, Articles, or Short Communications, whichever is appropriate, and will be collected into a bound Symposium volume by the organizers. Regular refereeing procedures will be applied.

A significant part of the studies to be presented will involve EPR as a tool. Topics to be covered in the invited talks include:

- Spectroscopy and matrix isolation techniques.
- Radical ions in photochemistry and radiation chemistry
- Synthetic applications of radical ions
- Radical ions on surfaces
- Radical ions in biological systems
- Radical ions in electrochemistry
- Quantum chemical techniques

The registration fee is \$250 for active participants. The cost for a first class hotel, centrally located, is approximately \$70/night, breakfast buffet included, but there are cheaper accommodations in student dormitories that can be arranged. The total number of participants is limited to about 100. Acceptance will be on a first-come, first-served basis. More details are available in a first circular that will be distributed to those interested in attending the conference. To obtain the circular, contact Mari Lofkvist, Secretary, RADICAL IONS 14, Department of Physics, IFM, Linköping University, S-581 83, Linköping, Sweden. For further information about the scientific programme please contact one of the chairmen: Anders Lund, Dept. Physics, IFM, Chemical Physics Laboratory, Linköping, Univ., S-581 83, Linköping, Sweden, FAX: 46-13-13-22-85, e-mail: ald@irm.liu.se; Sten Lunell, Dept. Quantum Chemistry, Box 518, Uppsala Univ., S-751 20, Uppsala, Sweden. Or communicate by FAX or E-mail: FAX: 46-18-50-24-02; E-mail: lunell@kvac.uu.se.

THIRD INTERNATIONAL WORKSHOP ON DOSIMETRY for RADIATION PROCESSING, Ste-Adèle, Québec, Canada, October 1-6, 1995.

This workshop will provide a continuing forum for examining all aspects of dosimetry related to radiation processing. All participants, whether novice or experienced, and whether involved in radiation processing of medical products, pharmaceuticals, polymers, foods, or other products, will benefit from the opportunity to interact with others from different backgrounds and disciplines. The informal format, with no published proceedings, encourages a free exchange of ideas and experiences between users, regulators and dosimetry experts. Participants will gain

information on current dosimetry practices, new and innovative techniques, and learn what the future requirements of dosimetry may be. Well-known invited speakers from around the world will provide the latest information on the workshop topics. Notable participants are expected from Austria, Canada, China, Croatia, Denmark, France Germany, Hungary, India, Italy, Japan, Netherlands, UK and USA.

There will be plenary sessions on topics of general interest, but the main focus will be small group "roundtable" workshop sessions on specific aspects of dosimetry and hands-on dosimetry measurements. These sessions will be scheduled at various times, and repeated so that attendees can create a program that best fits their needs and interests. An experienced workshop leader will chair each group to facilitate discussion and encourage input from all participants. A number of published ASTM standards on workshop topics will be distributed during the workshop to stimulate discussion. The Technical Sessions will include:

- Overview – Dosimetry Principles
- Overview – Selection, Calibration and Use of Dosimeters
- Dosimeter Selection, Calibration and Routine Use
- Dosimetry (Hands-on) Exercises
- Dose Mapping (Gamma)
- Dose Mapping (Electron Beam/Bremsstrahlung)
- Environmental Effects
- Overview – Uncertainties in Absorbed Dose Measurements
- Uncertainties in Absorbed Dose Measurements
- Industrial Applications of Dosimetry
- Dosimetry and Quality Assurance Programs
- Wrap-up

The Hôtel Le Chantecler is located in the scenic Laurentian Mountains north of Montreal. The hotel is fully equipped for indoor and outdoor recreational activities and is within easy walking distance of the quaint village of Ste-Adèle. This week in October is usually the best time for autumn colors in this region, and the weather can be quite cool. Separate spouses' activities such as sightseeing trips to Laurentian attractions and a shopping trip to Montreal are planned.

Space in the workshop is limited to 160. A Registration Fee of \$830 Canadian Dollars (or \$600 US Dollars) for the workshop and meals, excluding hotel accommodations, will be charged.

The registration form and additional information about the workshop may be obtained from:

Dr. Harry Farrar IV, Symposium Chairman, 18 Flintlock Lane, Bell Canyon, CA 91307, USA, ☎: 1-818-340-1227, FAX: 1-818-340-2132;

Rod Chu, Vice Chairman, Nordion International Inc., 447 March Rd., Kanata, Ontario, Canada K2K 1X8, ☎: 1-613-592-2790, FAX: 1-613-592-6937;

John Rickey, Vice Chairman, Far West Technology, 330-D S. Kellogg, Goleta, CA 93117, USA, ☎: 1-805-964-3615, FAX: 1-805-964-3162.

22nd ANNUAL CONFERENCE of the FEDERATION of ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES, Cincinnati, Ohio, October 15-20, 1995.

The FACSS meeting is one of the world's leading conferences in analytical chemistry, with over 1,500 participants and a program comprised of almost 1,000 presentations. This year, in addition to sessions on the core topics of atomic and molecular spectrometry, chromatography, and electroanalysis, the meeting will also feature sessions devoted to nanoscale analyses, biosensors for the 21st century, materials characterization, chemical analysis and neuroscience, challenges to environmental analysis, and issues facing the next generation of analytical scientists. Contributed original research papers are solicited in all areas of analytical chemistry. Titles should be submitted on a form obtainable from the FACSS National Office, 201-B Broadway St., Frederick, MD 21701-6501, USA; ☎: 1-301-846-4797; FAX: 1-301-694-6860. Submitted papers will either be 20-minute talks or be presented in poster sessions. (Note: The deadline for guaranteed acceptance of presentations has already passed; if late submissions are accepted, they are unlikely to appear in the printed program.)

INTERNATIONAL CONFERENCE on ELECTRON SPIN RESONANCE in ELECTRON TRANSFER and ORGANIC SOLIDS, Dresden, Germany, November 22-25, 1995.

The conference will be organized by the Institut für Festkörperforschung of the IFW Dresden. The topics include ESR in electron transfer reactions, ESR at fullerenes, ESR at conducting polymers and ESR as an *in situ* method. Presentations will be via invited lectures, short oral presentations and posters.

For further information, contact Dr. Lothar Dunsch, Institut für Festkörperforschung im IFW Dresden, e. V. Hemholtzstraße 20, D-01069 Dresden, Germany; ☎: 49-351-46-59-548; FAX: 49-351-46-59-313; E-mail: dunsch@ifw-dresden.d400.de.

POSITIONS WANTED

EPR Spectroscopist seeks a Postdoctoral Fellowship. Solid state physicist/chemist, 26 years old, Ph.D. 1994 (physics and mathematics), researcher at the Institute of Chemical Physics (Moscow, Russia). Research experience: Investigation of the microwave response in HTSC, conducting polymers (polyaniline), synthesis of byradicals with the help of mechanoactivation. Please contact: Dr. D.S. Tipikin, Institute of Chemical Physics, Russian Academy of Science, Kosygin Str. 4, 117977 Moscow, Russia; ☎: 7-095-939-71-85; FAX: 7-095-938-21-56; E-mail: kinet@glas.apc.org.

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 biopolymers, 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 Postdoctoral Fellowship Position. Semiconductor physicist, 32 years old, Ph.D. '88, research scientist 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; E-mail: lab24@isph.nsk.su; ☎: 38-32-354255; FAX: 38-32-354265; Telex: 133243 FONON SU.

POSITIONS AVAILABLE

Magnetic Resonance Spectroscopist Staff Position: Princeton University has an immediate opening for a Ph.D. level magnetic resonance spectroscopist knowledgeable in, e.g., EPR/ENDOR or solid state NMR or high resolution NMR spectroscopy. Primary duties involve maintenance of related instrumentation (hardware) and associated peripherals, including all spectrometer components, workstations, cryostats, probes, cavities, resonators and plotters; special projects in hardware design, electronic fabrication, training

of new users on basic as well as advanced techniques; scheduling and bookkeeping of multi-user instruments, educating students and faculty in new magnetic resonance methods and instructor for lectures on the theory of instrument operation; drafting of instrumentation proposals. The spectroscopist will fill one of two Professional Staff positions with complementary skills and overlapping instrument responsibilities in growing NMR/EPR facility (5 NMRs, 3 EPRs, 1 ENDOR). Send resume to Prof. Charles Dismukes, Operations Committee, Dept. of Chemistry, Princeton University, Princeton, NJ 08544. Princeton University is an Equal Opportunity/Affirmative Action employer.

Professor John Pilbrow, Physics Department, Monash University, has a position which could be either at the post-doctoral level or suitable for an appropriately qualified sabbatical visitor which could run from about nine months to one year, depending on seniority and negotiated salary level to carry out ESEEM and relaxation time measurements using a Bruker ESP380E FT/CW spectrometer. Person to have had experience in pulsed EPR (ESEEM etc.) in one or more of the following areas: transition metal ions in crystalline and non-crystalline solids, metal proteins, transition metal complexes.

In 1995 the group will consist of three Faculty members, two other post-doctoral fellows and three PhD students. Position could start almost immediately.

For further information contact Prof. John R. Pilbrow, Department of Physics, Monash University, Clayton, Victoria 3168, Australia; ☎: 61-3-905-3630; FAX: 61-3-905-3637; E-mail: j.pilbrow@sci.monash.edu.au.

Postdoctoral Research Position is available on an EU-funded project, to study the nickel-iron-sulphur enzyme hydrogenase, of which the structure has recently been determined. Experience with EPR or NMR or other spectroscopy an advantage. Training will be provided as necessary in spectroscopy, protein chemistry, and redox methods. There are opportunities for exchange visits to other research laboratories in the EU. The position is available immediately, for two years. Salary according to age and experience. Apply as soon as possible to: Prof. R. Cammack, Centre for the Study of Metals in Biology and Medicine, Division of Life Sciences, Campden Hill Rd., London W8 7AH, UK; ☎: 44-171-333-4264; FAX: 44-71-333-4500; E-mail: r.cammack@hazel.cc.kcl.ac.uk.

Help Wanted: A group in the Cancer Institute at NIH is working on a novel biological application of magnetic resonance spectroscopy. Some funding has been secured, and we are looking for an individual who might be interested to

help. We need a person with a good understanding of a modern spectrometer, particularly the analog and RF circuitry. Experience in RF design, hi speed signal switching, gradient coil design and the associated prototype execution and testing is highly desirable. No formal position has been established. The person could be on a postdoctoral or visiting scientist appointment, on an engineering or technician employment level or even part time as a consultant or outside contractor. Anyone who feels qualified and is interested in talking to us can contact me to exchange more information. All responses will be held in strict confidence.

Contact Rolf Tschudin, Bldg.5, Rm. B2-29, National Institutes of Health, Bethesda, MD 20892-0505, USA; ☎: 1-301-496-2692; FAX: 1-301-496-0825; E-mail: tschudin@nih.gov; CompuServe: 71543,751.

STA Fellowship Program — The Science and Technology Agency (STA), an administrative organ of the Government of Japan, established the STA Fellowship Program in 1988 in order to offer opportunities for promising young foreign researchers in the fields of science and technology to conduct research at Japan's national laboratories and public research corporations (excluding universities and university-affiliated institutes).

The Program is also a response to calls from the international community of science and technology for greater international cooperation through the exchange of promising researchers.

Since Oct. 1, 1989, the Program has been managed by the Research Development Corporation of Japan (JRDC), a statutory organization under the supervision of STA, in cooperation with the Japan International Science and Technology Exchange Center (JISTEC). JRDC also has the strong support and cooperation of Responsible Organizations.

For a brochure and more information about STA Fellowships, contact the Research Development Corporation of Japan, Science Building, 5-2, Nagata-cho- 2-chome, Chiyoda-ku, Tokyo 100, Japan. TEL:81-3-3507-3024; FAX:81-3-3581-1486.

"Postdoc International" — This organization groups together open job positions in the domain of research from laboratories around the world. Information on these openings is at the disposal of researchers through a computer server. Besides listings of numerous post-doctorate openings, the server also contains offers of permanent positions (senior researcher, laboratory director, etc.). Anyone having a computer account linked to an international network can access the server. Send e-mail to: post@docserv.saclay.cea.fr containing the text: "get index."

The file index contains the list of available files (the propositions are classed by country), as well as diverse information like conference announcements, financial programs for foreign sejours, and details on other computer networks of young physicists in the world.

This service is completely FREE, for both the seeker of information and the person who decides to insert an announcement on the list (send your text directly to the server with the command MESSAGE on the first line).

For more information, contact Clair Gautherin, President, Post Doc International, Service de Physique Nucleaire, Bat 703, Centre d'Etudes de Saclay, 91 191 Gif sur Yvette cedex; e-mail: gautheri@amoco.saclay.cea.fr.

EQUIPMENT & SUPPLIES EXCHANGE

AVAILABLE: VARIAN MODEL EM-500 EPR SPECTROMETER

Acquired at a surplus sale: Varian Model EM-500 Spectrometer (Serial Number 500032A01); will trade for "anything" or, at worst, give it away. The device appears to be in good shape, weighs ca. 400 pounds, is an X-band Impatt Diode device, and has a magnet with 4" diameter pole faces and 3/4" gap. If someone wants it they can pay for crating/shipping, or if local come get it with a small pickup truck. Varian has no records at all on this obsolete machine. From its size and simplicity it appears to have been designed as a student teaching aid. The serial numbers on the electronic parts suggest that it was made somewhere about 1965. For more information, contact Albert Bauman, A.J. Bauman Associates, 524 Oakdale Drive, Sierra Madre, CA 91024-1429, USA; ☎: 1-818-355-8698.

JEOL TE2000 SPECTROMETER

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

FOR OWNERS OF VARIAN & BRUKER EPR SPECTROMETERS

Micro-Now Instrument Company now has available replacement klystrons (new) for Varian 4500, E3, E4, Century Series and some Bruker spectrometers available at attractive prices. Contact Clarence Arnow, ☎: 1-708-677-4700, FAX: 1-708-677-0394; 8260 N. Elmwood St., P.O. Box 1488, Skokie, IL 60076, USA.

FOR OWNERS OF VARIAN EPR SPECTROMETERS:

(1) Field Scan Potentiometer; (2) Klystrons for Replacement; (3) Parts for Varian E-256 Electrolytic Cell; (4) Diodes for Varian E-101 & E-102 Dispersion Style Microwave Bridge Users; (5) Varian E-3, 9, 12 & E-104, 9, 12 CRT's :

(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 potentiometer 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 could 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, and E-104,9,12 users: I am arranging one large order for Varian X-Band Klystrons with Varian. If we have a sufficient quantity, Varian will supply with volume pricing. So I need to know your needs, that you would be willing to commit a purchase order to (at a later date). The pricing would probably be in the \$6000 range. I would extract a \$100.00 handling fee per order plus shipping for my time. Warranty period from Varian would be a 2-year shelf life plus a 3-year 12,000-hour prorated warranty (typical life 50,000 hours). Delivery times would be long term (6 months). If you need Q-Band or E-3 klystrons, let me know; these should be available as well. Prompt response will help in determining the Varian's pricing on this one-time order. Varian's quoted introductory pricing is \$7,000 for unit quantities and is subject to change. The volume price will only be available for a short period of time.

(3) I have the following parts to the Varian E-256 electrolytic cell, unused in factory wrappings: Varian PN 908721-02 Reference Bridge, with protective container; Varian PN 908721-01 Potential Bridge, with protective container; Varian PN 908723 Flat cell; Varian PN 908732

Reservoir upper half; Varian PN 908717 Reservoir lower half.

(4) 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, please contact me 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 difficult to obtain. The price would be \$150.00 each. 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 part. A purchase order would be required.

(5) I have a possible source for rebuilding E-3 crt's for the oscilloscope module. Let me know your needs in this area both now and for the future (I would like to know how many E-3's are still in operation). I will have one crt rebuilt shortly. Don't discard or break the old crt.

E-4;9; 12, E-104;9;12 crt's for the oscilloscope modules and the Varian NMR Gaussmeter are currently available new at \$255.00 ea. Buy one now for stock before they are discontinued. Stringing kits for the Varian recorder are available.

For information, contact James R. Anderson at Research Specialties, 5629 N. Maplewood, Chicago, IL, USA 60659. ☎/FAX: 1-312-728-6570.

WANTED: VARIAN MAGNET COIL

We are looking for a magnet coil for a Varian V-3400 9-inch magnet. We need the coil on the right-hand side (from the front). Please contact Shen or David at E-mail address "gashe@ttacs.edu" or call 1-806-742-3764. Jinmiao Shen, Physics Dept., Texas Tech Univ., Lubbock, TX, 79409, USA.

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.

WANTED: USED EPR/NMR ELECTROMAGNET

We are looking for a used 12" (or bigger) NMR/EPR electromagnet in a good operating condition. A used MRI imaging resistive magnet is also desirable. Please contact: Michael Chzhan, EPR Labs, Johns Hopkins University, Baltimore, MD, USA; ☎: 1-410-550-2438, FAX: 1-410-550-2448, E-mail: kppu@welchlink.welch.jhu.edu.

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.

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 lower cost is available from the University of Denver. Contact Richard Quine, University of Denver, Denver, CO 80208 USA; E-mail: rquine@diana.cair.du.edu; ☎: 1-303-871-2419.

AVAILABLE: TABLETOP NMR RELAXOMETERS

A portable (tabletop) NMR relaxometer, the "REKAR", has been developed by the Kazan Radio-Technical Institute. As the Innovation Fund of the Tatarstan Republic has provided funding to produce this instrument for sale, it is now available to users worldwide. REKAR is based on principles of pulsed NMR. Its main applications are express-analysis and testing of a wide variety of proton-containing substances. Computer and oscillograph outputs equip it for demonstrating the principles of pulsed NMR. The device is reliable, compact, fast, and universal. REKAR's flexibility and modular construction are key advantages.

Applications: The relaxometer can be used in different fields of science, education, as well as in medicine, oil, chemical and food industry:

Medicine: Blood analysis (viscosity, hematocrit, protein content in serum, degree of aggregation of erythrocytes, relative oxygen content, fibrinogen in plasm, colloid-oncotic pressure, osmomolarity); *Urine analysis* (viscosity, protein content, content of intracellular and extracellular water).

Oil industry: *Analysis* of oil products (humidity and content of high molecular products in oil and bitumen).

Chemical industry: *Analysis* of polymer materials (degree of hardening, crystallization and polymerization).

Food industry: *Test of food quality* (milk - fat content, protein content, acidity; meat - fat content, water content; agricultural - cereal, flour, sugar, etc.; humidity).

Electrodeposition: *Concentration* of main components of copper plating electrolytes, nickel plating, iron plating, metal paramagnetic ions in running and rising waters.

Basic REKAR Specifications:

Operating frequency, MHz	5.8; 10 (Optional)
Range of measurable relaxation times	2-3000 msec
Accuracy for T ₁ ; T ₂	± 3%; ± 5%
Automatic sample temperature range/accuracy	35-50 °C/± 0.1 °C
Field homogeneity, better than	10 ⁻⁴
Weight, 20 Kg, max	20
Dimensions:	310*210*265 mm (electronic unit); 265*210*235 (sensor)
Warranty on parts and labor	18 months
Special orders are welcome.	

A REKAR unit has been placed in the United States and is being modified for DNP (dynamic nuclear polarization) capability. It can be examined or demonstrated at the University of Illinois. For information, contact Dr. Yong-Min Chang, College of Veterinary Medicine, MRI Lab, 1008 W. Hazelton, Urbana, IL 61801, USA (E-mail: ychang@rlb6000.scs.uiuc.edu; ☎: 1-217-244-5670; FAX: 1-217-244-1475;) or the IERC (address on front page).

For more information, contact Prof. Boris M. Odintsov, Innovation Fund of Tatarstan Republic, Zurnalistov Str., 2a, Kazan, 420029, Russia; ☎: 7-8432-387331; FAX: 7-8432-761128; E-mail: root@kncran.kazan.su.

ANNOUNCEMENTS:

MAILING LISTS FOR SCIENTIFIC MEETINGS

If you are planning a scientific conference, you may contact an officer of the International EPR Society or the IERC (address on front page of this Newsletter) to obtain a list of the 1,000+ Society members for use in issuing invitations. If you would like to have preprinted mailing labels, Martha Moore, who provides secretarial support for the Society, can do this at cost -- approximately \$50.00 (includes cost of labels, postage and, if you wish, a disk copy of the list in ASCII format). Labels for the entire database (3,500+ members and non-members) would cost approximately \$175.00.

RECENT CHANGES IN PHONE AND FAX NUMBERS FOR INTERNATIONAL DIALING

We have been notified by Society members of two changes to standard phone numbers and will be entering these in our database as soon as possible.

1. When trying to reach numbers in Russian Federation, a zero must be used prior to the city code. For example, the city code for Moscow is 095, not 95 as shown in many of our directory listings.

2. When dialing to reach a number in the United Kingdom, a one (1) must now be used between the country code and the city code.

EPR NEWSLETTER

Volume 7, Number 2

Page 1

Summer/Fall, 1995

- Editor: R. Linn Belford, Urbana, IL (address below).
- Assistant Editor, Becky Callivan, Urbana, IL (address below).
- Typography: Martha Moore. *This, the official newsletter of the*
- *International EPR(ESR) Society, is supported by the Society, by corporate and other donors, and by three EPR/ESR centers:*

National Biomedical ESR Center,

Prof. James S. Hyde, Director. Medical College of Wisconsin, MACC Fund Research Center Building, 8701 Watertown Plank Road, Milwaukee, WI 53226, USA. ☎: 414-456-4008. FAX: 414-266-8515. E-Mail: cfelix@mis.mcw.edu
WWW: <http://141.106.72.102/BRI-EPR>

Biotechnology Resource in Pulsed EPR Spectroscopy,

Prof. Jack Peisach, Director. Albert Einstein College of Medicine, Dept. of Physiology and Biophysics, 1300 Morris Park Avenue, Bronx, New York 10461, USA.
☎: 718-430-2175. FAX: 718-430-8935.
E-mail: peisach@aecom.yu.edu
WWW: <http://spin.aecom.yu.edu>

Illinois EPR Research Center (IERC),

Prof. R. Linn Belford,* Director; Prof. Harold M. Swartz,† Co-Director at Dartmouth; Prof. Robert B. Clarkson,* CoDirector; Prof. Peter G. Debrunner, Assoc. Director,* Prof. Mark J. Nilges,* Asst. Director, Dr. Alex I. Smirnov,* Laboratory Manager at Urbana, Dr. Tadeusz Walczak †.

* University of Illinois at Urbana, 190 MSB, 506 South Mathews, Urbana, IL, 61801, USA.

☎: 217-244-1186. FAX: 217-333-8868.

New E-mail address: ierc@uiuc.edu or

rlbelford@uiuc.edu

† IERC satellite site for EPR in viable biological systems at Dartmouth College, Hanover, NH, USA.

☎: 603-650-1955; FAX: 603-650-6525;

E-mail: harold.swartz@dartmouth.edu]

WWW: <http://ierc.scs.uiuc.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.

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

HYDE NAMED TO RECEIVE THE ZAVOISKY AWARD

Following extensive nominations from the international community of EPR scientists, the International Zavoisky Award Committee is delighted to announce that the E. K. Zavoisky Awardee for 1995 is Professor Dr. James S. Hyde (National Biomedical ESR Center, Milwaukee). He will be awarded the Prize at the annual Workshop "Modern Development of Electron Paramagnetic Resonance" to be held in Kazan 27-30 September, 1995.

Prof. J.S. Hyde is distinguished for the laureate's work in electron paramagnetic resonance and, in particular, his contribution to instrumentation and methodology of electron paramagnetic resonance spectroscopy. A further citation of his work will appear in a forthcoming issue of "Applied Magnetic Resonance."

Prof. Kev. M. Salikhov
Chairman, Zavoisky Award Committee



Comments honoring Professor Lev Blumenfeld upon the award of the International EPR Society Silver Medal in Biology/Medicine

The significant contributions of Professor Lev Blumenfeld (Russian Academy of Sciences, Moscow) to biomedical EPR are too numerous to list. They were reported in over 300 publications and summarized in four books. He was one of the pioneers of biological and chemical EPR studies. In 1955 he discovered free radical EPR signals in freeze-dried tissues of animals and plants. His early studies drew the attention of biophysicists, biochemists, and physiologists, and promoted the study of the role of paramagnetic intermediates in intracellular metabolic processes. He worked with both purified systems such as enzymes and intact biophysical entities such as mitochondria. He and his colleagues made decisive contributions to the identification of free radicals in metabolizing tissues. He brought the rigor of a physicist to the biomedical applications of EPR, thereby advancing the field and setting a standard for those who came to the field later.

Some of the specific studies for which he is noted include the identification of semiquinone radicals in functional cells, paramagnetic intermediates in enzyme systems, and studies of iron-sulfur proteins and their relation to redox metabolism. He made some of the earliest studies of the reaction of nitric oxide with proteins.

Over the past two decades his interest has focused on energy transduction in enzymes and biomembranes. His interests have even extended to EPR in ceramic superconducting materials.

Professor Blumenfeld has also contributed to the field by training many of the leaders of EPR spectroscopy (too many to list here), including the winner last year of the Silver Medal for physics/instrumentation, Professor Wojciech Froncisz.

Several colleagues contributed the comments that were combined for this tribute, which was read at the 18th International EPR Symposium (Denver, July, 1995) by Professor Sandra S. Eaton on behalf of the International EPR (ESR) Society.

Unfortunately, Professor Blumenfeld could not extend his travel in the USA long enough to attend this meeting. Happily, his son was able to attend and present his award address in his place.

Denver, Colorado, USA, July, 1995

FROM THE EDITOR

Reminder: The IES Awards Committee begins its work in January, so please send your nominations for awards before the end of the year! See *IES Affairs* below for details.

I was impressed and delighted with the tone and substance of the events at the 18th International EPR Symposium (Denver, July, 1995) honoring Sam Weissman (Professor at Washington University, St. Louis, Missouri), as the Gold Medal Awardee of the International EPR(ESR) Society! Sam's illustrious former student Jim Norris (University of Chicago) was the general master of ceremonies for these events. First, after the award presentation, Sam delivered his fascinating Award Address, "Getting Started in EPR," in his customary terse, pithy, and modest manner. Next, there was an all-day Gold Medal Award Session featuring the following talks by an

impressively stellar group of associates and former students of Sam Weissman: "Microwave Frequency Dependence of CIDEP" by Noboru Hirota, Kyoto University; "Angle Selected ENDOR Spectroscopy; EPR Spectra as 3-Dimensional Energy Surfaces" by Robert Kreilick, University of Rochester; "Applications of FT-EPR in the Study of Mechanisms of Photochemical Reactions," by H. van Willigen, University of Massachusetts, Boston; "Probing Electron Transfer with Low and High Field EPR," by James Norris, University of Chicago; "EPR and DNP at High Magnetic Field" by Robert Griffin, Massachusetts Institute of Technology; "ESR of Photoexcited Alkali-Metal Solutions. The Way It Is" by Haim Levanon, Hebrew University, Israel; "Light-Induced Nuclear Coherences in Photosynthetic Reaction Centers" by Gerd Kothe, University of Freiburg, Germany; "From Conventional to Echo-Detected Transient Nutation of the Photo-Excited Triplet State" by Tom Lin, Washington University, St. Louis; "Transient EPR with No RF Pulse - A Fast Switching Experiment" by David Sloop, Washington University. The gala award banquet featured after-dinner kudos and reminiscences by Clyde Hutchison recalling Sam's student and early days at the University of Chicago. We heard about Sam's keen intellect and other qualities, including his famed economy of written language; his doctoral thesis was said to be the shortest ever to have been produced and accepted at the University of Chicago, so short that filler pages had to be added to make it possible to bind. We then heard from several former members of Sam's research laboratories who reminisced about the earlier and not so early days there. A recurring theme was Sam's patience, good humor, sharp mind and insight, and splendid success in fostering the development of his students and postdoctoral associates. This was a wonderful occasion for all of us. Throughout the entire symposium, Sam impressed me with not only his wit, but his attentiveness and contributions to all the scientific proceedings. He sat in the front row through all the talks, the whole week, and contributed insightful comments and questions. Sam Weissman is a model for all of us, but he is one of a kind - good to emulate but impossible to duplicate!

Also enjoyable at the same conference was the awarding of the IES Young Investigator Awards for 1994 and 1995 (see *Awards* report in *IES Affairs* section below). The two

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award addresses - Dr. Mustafi's, "Application of Angle Selected ENDOR for Structure Determination", and Dr. Britt's, "ESR-ENDOR Studies of Paramagnetic Centers of Photosystem II", were very well received and, for me, confirmed the soundness of the Awards Committee's choices.

R. Linn Belford
Urbana, Illinois, USA, September, 1995

◆ **IES AFFAIRS** ◆
**ANNOUNCEMENTS AND
REPORTS FROM THE INTER-
NATIONAL EPR SOCIETY**

From the President —

At this time of year, near the end of the conference season, I like to look back on what we have accomplished in the past twelve months. The Society has been associated with three major meetings, EPR-95 and ISMAR in Sydney, and the Denver meeting whilst Hal Swartz and I have kept the profile of the Society high at several others. One result has been an increase in the number of our new members, but this has been disappointingly offset by the failure of some of our existing members to keep up their subscriptions. Much of this has resulted from difficulties in exchange of many currencies into US dollars, and so we have made, and are still making, strong efforts to establish more regional treasurers to whom dues may be paid in local currency. A cash flow is essential for the continuance of the Society and we should be grateful for any more volunteers willing to fulfil this role in countries in which no local treasurer exists at present. Similarly, we hope existing members will continue to bring the existence of the Society to the attention of their colleagues. Many new ESR scientists have started work since the Society was founded, and we hope that they will join too; many will have seen the Newsletter in the groups in which they are working, and if so I feel sure they will wish to continue receiving it. Although the Officers of the Society have the clearest duty to maintain and increase membership, both individually and corporately, we always appreciate your help, and indeed depend upon it.

The Society continues to associate itself with international conferences whilst running none of its own. This policy results from the fact that several ESR societies pre-existed our own, and we have no wish to compete with them for conferees, but see ourselves rather as a central enabling and helping body. By adopting this approach we supply different services to the community than do the local societies, and we rejoice in having many of their members amongst our own. The truly international nature of the Society has continued to evolve throughout the past year in a very satisfying way for your Officers, who have always had this as a major goal. We have committed the Society to co-operation in the next meeting of the European federation

of ESR Societies in Leipzig in 1997, and to the next (joint) meeting of the ISMAR and AMPÈRE groups in Berlin in 1999, where strong local ESR representation will ensure that ESR plays an important role.

Two other matters which give me great satisfaction are our collaboration with the UK Society and the Russian one in awarding the major prizes of our subject (The Bruker, the Zavoisky and our Gold), and in our successful introduction of Fellowships. In the former case we are indebted to our colleagues in the U.K. and in Russia for their cooperation. In the latter, five scientists of the highest international esteem, Profs. Abragam, Bleaney, Hutchison, Prokharov and Weissman, have honored us all by accepting their awards. We intend to maintain this extreme standard of election.

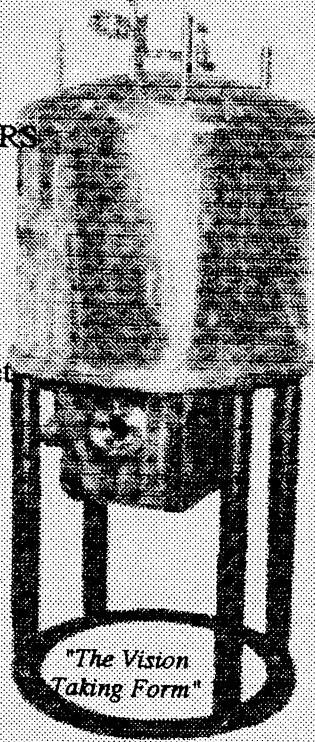
At present Hal Swartz as Chairman of the Nominating Committee is giving much thought to who might replace your present Officers whose term of office is approaching its end. The Committee intends to make recommendations to the posts but the choice is yours, and we should be pleased to receive any suggestions that you might have. We do intend to suggest small changes in practice, for example to provide additional continuity between one bunch of Officers and the next, but all the posts will remain.

The Society operates due to the efforts of many people who go unsung in our reports simply because they do everything asked of them, and more, purely to help us all. This includes our wonderful helpers at the IERC, Linn, Becky and Martha, the regular contributors to the

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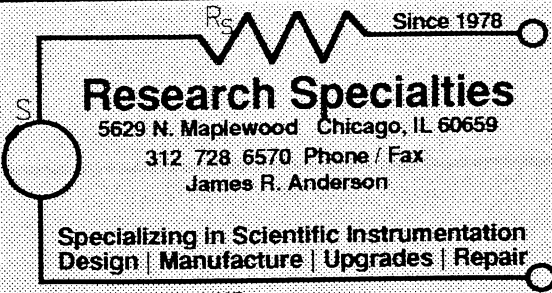
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Newsletter, the Chairmen of all the sub-committees, and, if I may mention one specific name since this edition contains so much of his work, Peter Gast, who sets up the database each year for the annual directory issue. All of this would be of little use without the continued support of our Corporate Sponsors, which we greatly appreciate. We hope our members think first of them when purchasing, which I am sure they do from the number of people who tell me how useful it has been to find sources of equipment, etc. through their advertisements in the Newsletter.

As ever, we should be pleased to hear of any suggestions for changes in the way we run the Society from you, and any criticisms you would like to make. We are very conscious that with such an international membership we might cause offence without intending to, and we should far sooner have criticism in the open through the Newsletter than to carry on ignorant of it. This applies, of course, to both corporate and individual members.

Keith McLaughlan.

Awards

I am pleased to announce that the Young Investigator Awards of the IES have been made as follows:

1994: Dr. Devkumar Mustafi, Dept. of Biochemistry and Molecular Biology, Cummings Life Center, Univ. of Chicago, 920 E. 58th St., Chicago, Illinois 60637, USA. Interests: largely ENDOR applied to Biology. Refs: Marvin Makinen, Clyde Huchison, N.D. Chasteen, David Doetschman.

1995: Prof. R. David Britt, Dept. of Chemistry, Univ. California, Davis, CA 95616, USA. Interests: Pulsed ENDOR, primary mover of pulsed EPR in his area, already with world recognition at conferences, etc. Ref: Gus Maki.

Important: Nominations for all the awards of the IES for the coming year are due January 1, 1996.

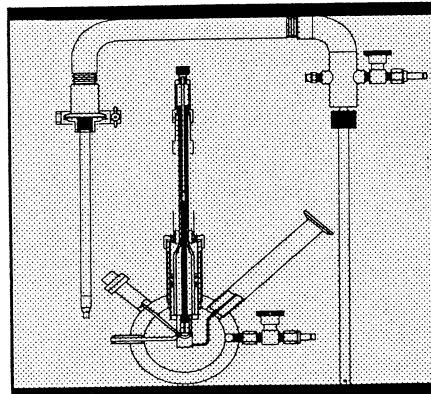
We repeat here the Society's award policies: Awards are not restricted to IES members, but the committees may take membership into account when deciding on the award winners. Agreement has been reached between the British and Russian Groups and ourselves to co-operate in the award of the Bruker and Zavoisky Prizes and our Gold Medal Award each year, with each group invited to make input into the selection of each, but with the final choice left to each group. The area of research interest is to rotate between the groups each year, with the loosely-interpreted categories, chemistry, physics and instrumentation, and biological sciences (including medicine), these are meant to be interpreted liberally and not to be restrictive.

In the coming year (1996), the IES Gold Medal award will be in Physics and/or Instrumentation, the Bruker in Chemistry, and the Zavoisky in Biology and/or Biological Sciences. Prof. Larry Berliner, continuing Chairman of the Gold Award committee, will welcome nominations for this.

Gold Medal: 1996 Gold Medal, recognizing benchmark contributions to EPR spectroscopy in chemistry. Nominations to Prof. Larry Berliner.

Silver Medals: One each in the general areas of Chemistry, Physics/Instrumentation, and Biology/Medicine. To propose names, please send your suggestion(s), or preferably full nomination(s), to the appropriate Silver Awards Sub-committee(s): *For Physics and Instrumentation* - Jim Hyde, Chair; John Pilbrow, George Feher, & Jan Stankowski. *For Chemistry* - Bruce Gilbert, Chair; N. Hirota, Jim Bolton & Kev Salikhov. *For Biol./Medicine* - Harold M. Swartz, Chair; Marjeta Sentjurs, Hideo Utsumi & Tadeusz Sarna.

Young Investigator Awards: One Young Investigator award each year; "young" is defined as being under 35 on



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January 1 of the year the award is made. Send nominations to Prof. Keith McLauchlan.

Before the end of 1995, send nominations for 1996 award to Prof. Keith McLauchlan.

Fellows of the Society

The IES has created Fellowships to recognise truly outstanding contributions and achievements in electron paramagnetic/spin resonance among these scientists (hopefully, IES members) who are either retired or are close to retirement. (Fellows of 1995: Anatole Abragam, Brebis Bleaney, Clyde Hutchison, Aleksandr Prokhorov and Samuel Weissman). The highest international standards are to be applied to the recognition of those worthy of this distinction, and their formal connection with the Society will enhance its own image. Nominations for consideration by the Committee are to be sent in confidence to Keith McLauchlan by January 1, 1996.

THE COMPUTER CORNER

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

The EPR Computer Corner is a regular feature of the EPR Newsletter. It is managed and edited by Reef (Philip D., II) Morse (reef@xenon.che.ilstu.edu), Graeme Hanson (graeme@cmr.uq.oz.au), Keith Madden (madden@marconi.rad.nd.edu), Dick Cammack (udbc033@hazel.cc.kcl.ac.uk), and Dave Duling (duling@niehs.nih.gov). Items for this column may be sent to any of the above authors. Submissions may be edited for publication.

Spin Trap Database

by Dave Duling, NIEHS-Biophysics Information Systems and Networks.

In recent weeks we have received several inquiries regarding the status of our freely available Spin Trap Data

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Base (STDB), a compendium of published spin trap parameters. This report will discuss the current and future states of the database including the possibility and organization of a worldwide repository of spectroscopic data.

The STDB originated with a paper published by Gary Buettner in 1987 listing spin adducts derived from DMPO, PBN, MNP and other popular spin traps. In 1988 Anson Li created a computerized version of the database which allowed for interactive search and retrieval of data. For the next six years, Dr. Li improved upon the computer program as thousands of additional records were added to the database. The STDB now has data from over 9,000 published experiments. In addition, we have distributed a DOS version of the database program to over 100 researchers worldwide; the current version is numbered 6.0.

In 1995, we unveiled the Internet World Wide Web (WWW) version of the database. This version applies the powerful data distribution capabilities of the WWW to EPR spectroscopy. With the WWW, a researcher can distribute text, graphics, or virtually any other data to literally thousands of other people in a matter of minutes. The WWW has caused explosive growth in the use and commercialization of the Internet to the point that the 'net is now a largely self-supporting enterprise not dependent on government support. Currently, the number of WWW sites and quantity of content is so large as to be immeasurable. Most people with access to an Internet connection can make

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full use of the WWW with a "browser" program such as the Mosaic software from the University of Illinois' National Center for Supercomputing Applications (NCSA) or the Netscape software from Netscape Communications. Both packages are readily available on Internet archives.

This new version of the STDB is a service that runs on our WWW server and is available to anyone on Internet with a WWW browser using any computer such as a Macintosh, MS-Windows, or a UNIX workstation while the latest "old" version required a DOS computer. Also, by using one version of the database on our host computer, researchers can be assured they are retrieving the latest information available. The new STDB is made up of WWW pages that are forms for data entry. A user will see fields for: Keywords, Solvent, Molecule, spin trap type, and spin trap hyperfine values. Keywords can be text such as "uv", "NADPH", "microsomes", etc.... The user then selects SEARCH and after a hopefully brief wait will see a page of summary results. The index number for each result is linked to the full journal reference. For instance, a search for solvent=AQ, molecule=OH, spin trap=DMPO returns 258 data records. Expanding the search to any trapped molecule in aqueous solution yields 883 records. The host computer can execute this search in literally milliseconds so that the only limit on your search speed is the network connection from your site to ours. In addition, users can submit new data using the WWW. Another page has fields for entering the journal reference and experimental results. The data will then be reviewed by LMB staff for errors and then added to the database.

However, the WWW STDB is only scratching at the surface of potential data distribution. There is now no reason the data should be restricted to spin trap experiments. In fact, we have widened the organization of the system to include any magnetic resonance data. The new Magnetic Resonance and spin trap Data Base (MRDB) can accept actual data from any form of experiment. Users can submit NMR, mass spectrometry, IR, UV-vis, even a manuscript text, in fact, any form of data along with a textual

description. The textual description will be used to index the database which can later be searched and the actual experimental results retrieved. We have loosely termed this new system the 21st century Landolt-Bornstein. Imagine being able to search a worldwide database for all experiments on Fullerene and retrieve NMR data from Australia, EPR data from Europe, or IR data from India. Currently, we have organized the mechanism to receive new data and are working on the mechanisms for indexing and distributing the data. We hope to have trial data sets available by the end of 1995 and to have the system fully usable in the first quarter of 1996. In the meantime, we need users to try out the system of uploading actual data and report their impressions of the organization and potential usefulness of the system.

The WWW address for the system is: <http://alfred.niehs.nih.gov/LMB/spectra/mrdb/mrdb.html>. Select "Spin Trap Data Base" from the list of options.

EPRSim XOP: Powder and Isotropic EPR Simulation Operation for Igor Pro.

Requires: Macintosh computer with a math co-processor and Igor Pro software.

John Boswell at the Oregon Graduate Institute of Science and Technology, has developed an XOP (external operation) for the Macintosh graphing and numerical analysis program, Igor Pro. His XOP, EPRSim, implements the QPOW powder EPR simulation code of Nilges, Belford, et al. (IERC), and can also generate isotropic spectra. He has successfully used the XOP to simulate the spectrum of PHM (a type-II copper protein), as well as the spectrum of a DMPO-S (thyl) radical (spin trapped).

Versions for 68k and PPC Macs are available, as is a "fat" version that will run on either platform. He has also put together a demo experiment that shows how to use the simulation routines, and gives sample input and output. You can find the XOP and demo experiment, as well as an online example of the simulation output using a web browser such as Mosaic or Netscape. Set the http: to:

http://www.cbs.ogi.edu/~boswell/XOP_page.html

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or, you may obtain them via anonymous ftp from amethyst.cbs.ogi.edu in the directory pub/xop. The files are binhexed, self-extracting archives. The program is email-ware. If you use the program, please send John email with any kind of feed-back. John's address is:

John Boswell, Oregon Graduate Institute of Science and Technology, Department of Chemistry, Biochemistry, and Molecular Biology, PO BOX 91000, 20000 Walker Rd, Portland, OR 97291-1000; ☎: 503-690-1086; E-mail: boswell@amethyst.cbs.ogi.edu or knight@grafton.dartmouth.edu

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EPR SPECIALIST VIGNETTES

Edited by
Arthur Schweiger

In this issue, we are pleased to feature, from Tbilisi, Georgia, an account by Dr. T. I. Sanadze of the interesting phenomenon of discrete saturation:

DISCRETE SATURATION

by Tengiz I. Sanadze

Tbilisi State University, Chavchvadze av. 3
Tbilisi 380028, Republic of Georgia

In spring 1964 we observed at Tbilisi State University a strange behavior of EPR lines under pulsed saturation. Instead of the expected single hole, a large number of holes (Fig. 1) were burnt into the EPR line at low temperatures. It was evident that this hole spectrum was related to hyperfine interactions between the electron spin and the neighboring nuclear spins, but the cause for their formation still remained an enigma.

At that time we knew about the attractive results of Feher and Gere [1], who also observed a hole spectrum, which they ascribed to spectral diffusion. But our observations were absolutely opposed to those described in ref. [1]. In Feher's case the intensity of the side hole spectrum increased with the duration of the saturating pulse. In our investigations however the spectrum was formed immediately after the pulse and only spread in time by usual cross-relaxation processes within the line. Moreover, at low concentrations of the paramagnetic centers (e.g. for free radicals in polyethylene at low irradiation doses in the reactor) the burnt hole spectrum was "frozen" for a long time. So in our case spectral diffusion could be ruled out; we therefore called this phenomenon "discrete saturation" (DS).

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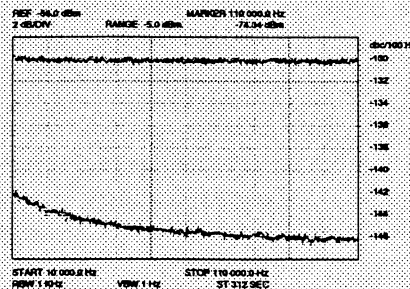
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The spectrum illustrated was taken with a Varian weak pitch sample in a TE102 cavity under the conditions specified in the Varian E Line Series unmodified (E102/E100 bridge) instruction manual. Signal to noise ratio represented is 245:1. A 2.5 conversion factor was used to convert rms noise to P-p noise. The weak pitch sample had a 663 multiplication factor. Without the multiplication factor, the signal to noise would be 369:1.



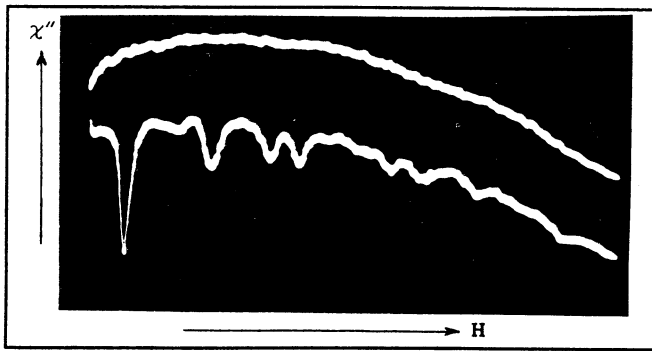


Figure 1. Oscilloscope photograph of the DS spectrum of Yb^{3+} trigonal centers in SrF_2 with B_0 along $[1 \bar{1} 2]$ and the shape of the same portion of the EPR line without saturation (above).

Even in our first publication [2] which appeared at the urgent request of Academician E.K. Zavoisky, we pointed to the main cause of DS: The change of the direction of the effective magnetic field acting on a nuclear spin as a result of electron spin transitions. Here the probability of the electron transitions with and without nuclear spin reorientations become of the same order of magnitude.

At that time, however, we considered only the possibility of the reorientation of a single nuclear spin. Though this situation was very simple from the mathematical viewpoint (the probability of independent events is equal to the product of their probabilities), in practice it was difficult to overcome the psychological barrier that forbidden transitions should be responsible for the phenomenon. Who would even assume that the lines of the fluorine hyperfine structure (HFS) in the EPR spectrum of U^{3+} in CaF_2 , observed on the oscilloscope, corresponds to the simultaneous reorientation of all the eight fluorine nuclear spins surrounding the paramagnetic center? However having overcome this psychological barrier we could easily explain the DS spectra [3].

Thus, let us suppose that we saturate a particular narrow region in an EPR line which is formed by the electron-nuclear transition $(+1/2, M) \leftrightarrow (-1/2, M')$, where $\pm 1/2$ are the electron spin projections and M and M' are the values of the total spin projection for equivalent nuclear spins ($I=1/2$) close to the paramagnetic center. This saturated portion will correspond to the central hole. In this case all the transitions $(+1/2, M) \leftrightarrow (-1/2, M^*)$ and $(-1/2, M') \leftrightarrow (+1/2, M^*)$ will be partially saturated. Here M^* denotes any value of the total projection of the surrounding nuclear spins which form the portion of the EPR line in the vicinity of the central hole. Thus we obtain two independent hole subsystems which are superimposed on one another and are connected with the upper $(+1/2)$ and the lower $(-1/2)$ electron spin states. It can be shown that the observed DS spectrum represents the shape of the spin packet burnt in the EPR line. The entire hole spectrum appears together with the central hole and its intensity increases with pulse power and pulse duration. In other words, the DS spectrum reveals all transitions that are connected with the saturated portion of the EPR line with resolved or unresolved HFS.

For the first time the DS technique was used to investigate fluorite-type single crystals with U^{3+} impurity (where the DS phenomenon had been discovered). In this system which shows a well-resolved fluorine HFS the paramagnetic ion is surrounded by eight equivalent fluorine nuclei. While earlier the analysis of the complex HFS looked like "reading the tea leaves", the DS technique significantly simplified this problem. It remained only to "read" the DS spectrum and enter the data into a computer, which gave a curve of the expected lineshape in full agreement with the experiment. It was found that the observed fluorine HFS components of U^{3+} in CaF_2 are grouped according to the selection rules, i.e. each of them has its own selection rule for the reorientation of the total nuclear spin projection M [4].

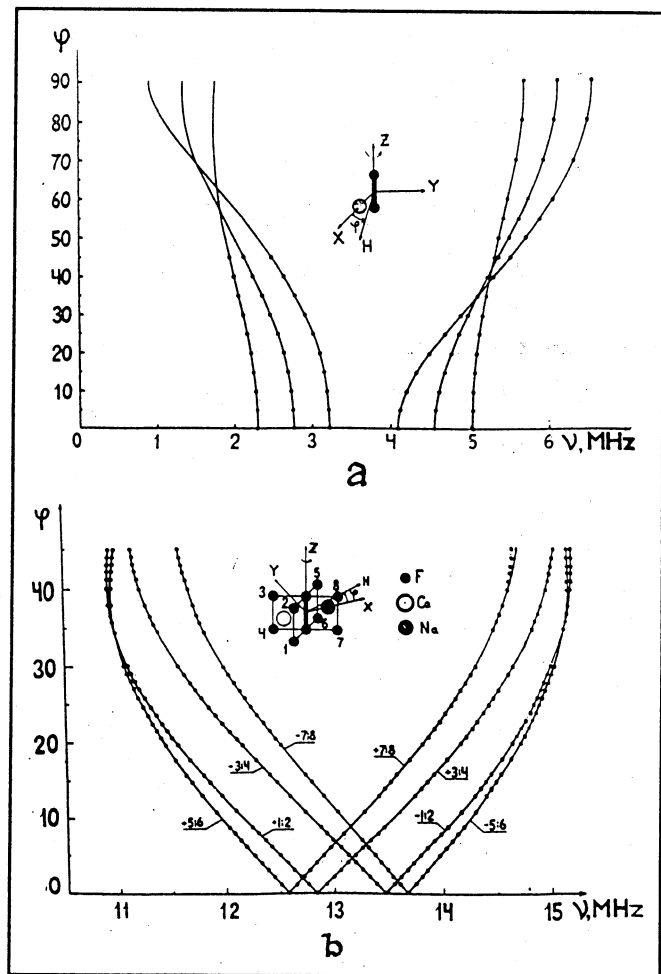


Figure 2. Angular dependence of RFDS spectra of Vka centers in $\text{CaF}_2:\text{Na}$ perpendicular to the F_2 - molecule axis. a) sodium transitions, b) fluorine transitions.

The resonant perturbation of a DS spectrum by a radio frequency (rf) pulse, followed by a microwave pulse predicted in 1971 [5] was demonstrated experimentally in our laboratory one year later [6]. As a result of rf irradiation one of the independent subsystems of the DS holes is always reduced in intensity and some new holes may appear. This

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effect allows the direct determination of the electron spin states. The method which we call RFDS, represents one of the pulsed version of ENDOR (DS-ENDOR). As an example we mention the application of RFDS in an investigation of V_{KA} hole centers in $CaF_2 : Na$ [7]. Fig. 2a shows the angular dependence of the sodium transitions in the RFDS spectrum in the plane normal to the V_{KA} center axis. The corresponding angular dependence of the eight neighboring fluorine nuclei is shown in Fig. 2b. Experiment and theory which also considered the quadrupole interaction of the sodium nucleus are found to be in excellent agreement.

For many years DS spectroscopy has been applied only by a few groups of physicists with limited technical potentialities. The situation has however significantly changed in the last couple of years by applying Fourier transform spectroscopy to DS and RFDS [8,9]. In these approaches the entire hole spectrum is observed via the FID that follows a short microwave pulse rather than by a rapid field scan. It should be emphasized that in recent years a commercial multi-purpose pulsed EPR spectrometer has become available, so that the application of powerful pulse methods like DS or RFDS has now become straight forward.

The other branch of the hole burning spectroscopy revealed in ref. [1] has also undergone an interesting evolution. It was further developed [10] and brought to perfection in a recent work under the beautiful acronym FORTE (forbidden-transition-labelled EPR) [11] which is a surprisingly exact reflection of its essence. When the intensities of "forbidden" transitions become small, the DS spectrum degenerates into a single hole. In such cases the

forbidden transitions can significantly be enhanced in intensity by saturating these transitions (or inverting the corresponding level populations) by a strong microwave pulse.

In conclusion it is definitely right to say that the various methods used in hole burning spectroscopy owing to their simplicity and high informative capability will find wide application in EPR for the study of hyperfine interactions.

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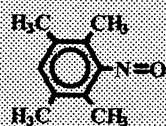
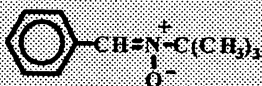
Building The Perfect Beast

Chris Bender

NIH Biotechnology Resource for Pulsed EPR

IDENTIFYING INSTRUMENTAL ARTIFACTS IN ECHO MODULATION SPECTRA

The spectrum obtained in an electron spin echo modulation experiment is a Fourier transform of the time-dependent variation of the echo amplitude. The conventional

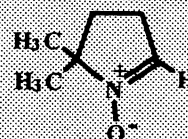
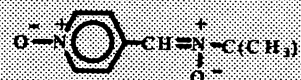


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method of recording the time domain data is by using a gated integrator or boxcar. This device samples the voltage (there is also a version that measures current) for a short time interval; because the shape of the echo is not square, the integrated voltage is the measured captured parameter. Most

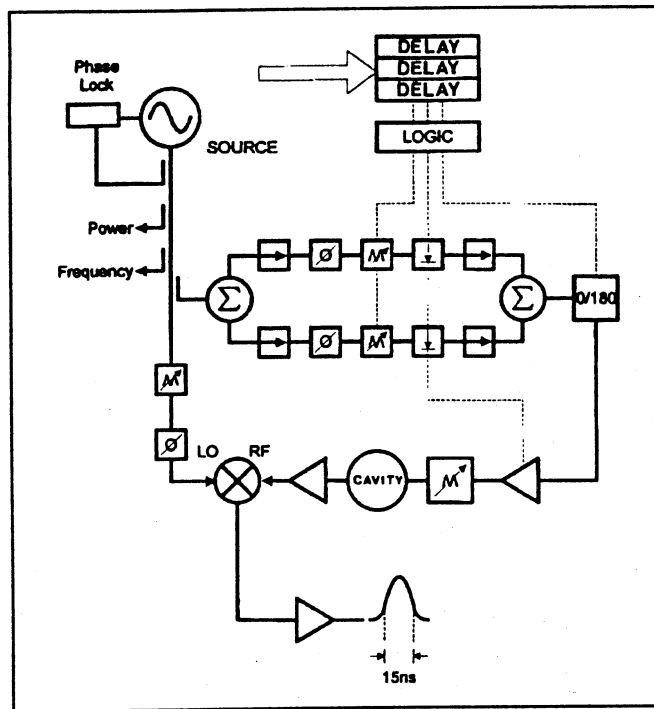


Figure 1: Pulsed EPR spectrometer layout. The reference arm is indicated by the direct transmission line between source and LO port of mixer and includes a variable attenuator and phase shifter as circuit elements.

of us use a homodyne detection system. The measured signal (echo) is received by one input (RF port) of a double balanced mixer and down converted to the DC voltage that is sampled by the boxcar. The down conversion process requires that a continuous wave rf source be input at the so-called LO port of the double balanced mixer. When the signals at RF and LO are at the same frequency (which they should be in a conventional spectrometer), the DC voltage at the IF port will vary according to: i) amplitude of signal at RF; ii) amplitude of signal at LO; phase coincidence of RF and LO signals.

The layout of the spectrometer is reproduced in Figure 1. The reference arm is the source of cw radiation at the LO port, and the RF port receives the pulsed echo signal via the cavity. The length of the transmission lines differ, however, and there is no *a priori* way to make the lines operate in phase without inserting a phase shifter (i.e. an adjustable line) in the reference arm. Ordinarily one sets up an experiment by adjusting the phase of the reference arm to maximize the signal at the IF port. This is what you are doing on a conventional spectrometer bridge that has a reference arm. Figure 2 illustrates the effect of reference arm phase on the echo amplitude observed on our pulsed

spectrometer; I also have an attenuator on my reference arm, and the inset illustrates the echo amplitude as I dial through the range of attenuation.

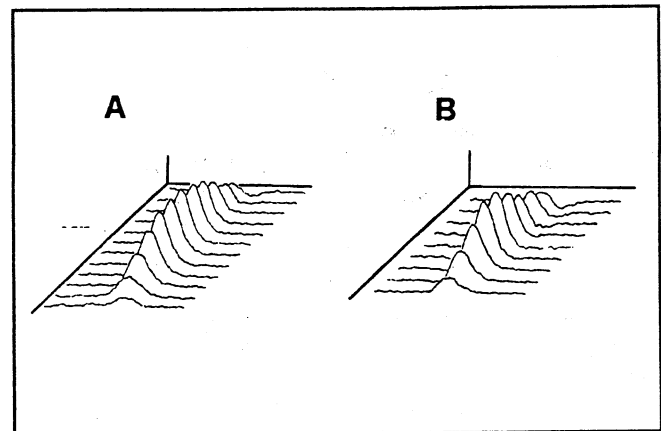


Figure 2: Variation of echo intensity as a function of mixer LO port parameters. A) Stepping through phase. B) Stepping through power.

Given an understanding of how the receiver works, it should come as no surprise that if the phase shifts during the experiment, one will observe spurious echo 'modulation'. To cite one very simple example: my sample cavity sits in liquid helium and the waveguide feeds to the cavity pass from a region of (mostly) helium gas into the liquid helium. So my transmission lines are partially loaded with a dielectric (that section of the waveguide that is filled with liq He). As the helium boils off, the level drops and the dielectric loading of the transmission lines changes. This, in turn, leads to a phase shift, and during the course of a day's operation I'll have to readjust the reference arm phase. This 'drift' in phase is usually benign because it's monotonic and manifests itself as an artificially accelerated phase memory loss on slow acquisitions. I'd worry only if I was trying to accurately measure relaxation times.

What does worry me is an apparent cyclic phase shift in my electron tubes, namely the klystron and/or the traveling wave tube, that can be detected when I am recording data at high receiver gain. I have sometimes noticed that when my 'true' modulation is shallow and short-lived there is a very low frequency component that makes the modulation trace look like a whip photographed in mid-snap on data collection series of 30 min. (if I let the computer collect stationary echo amplitudes for >2hr I will record a cyclic waveform); the modulation is not pronounced, but clearly the trace is not decaying monotonically as you would expect. What made this suspicious when I first saw it was the fact that everything else died out in the first 5 μ s, and here was this sole component lingering on seemingly forever. The suspicious modulation showed up in the FT spectrum as a low frequency peak. I should mention that I also observe the spurious feature in 'prettier' modulation that is deep; it's just less obvious.

I can't seem to rid myself of this apparent artifact despite attacks on the traveling wave tube amplifier and the

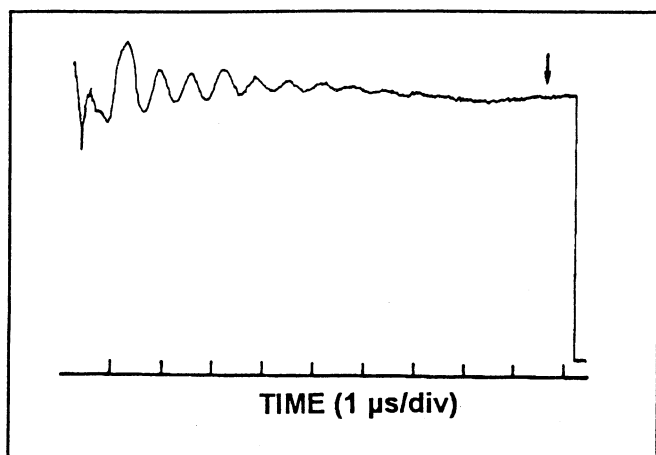


Figure 3: Three pulse echo modulation of rusticyanin at $g=1.98$; 1000 time series points are collected sequentially with 100 samples of integrated echo intensity per point. Data collected at 25 - 30 Hz (>1hr for experiment). The phenomenon referred to in this note is indicated by the arrow.

klystron/phase lock. I did, however, figure out a way to identify an artifact that is instrumental in origin when such suspicious modulations appear. The idea is basically this: the instrumental modulation has some oscillatory period, call it τ_{BAD} , that is independent of the spin system but dependent on the data acquisition rate. If you sample the echo at the same rate (say 100 Hz) and same number of points (1000 on our spectrometer), the 'bad' oscillation will always appear with the same waveform on the monitor. In other words, you can change the step size (increment of change in the pulse separation) in your spin echo experiment (e.g. 5 vs. 10 ns); the spin system is unaffected and the echo modulations will compress or expand accordingly in the time domain because the time scale changes. From the standpoint of the data acquisition, however, the time scale has not changed (you're still collecting 1000 points at 100 Hz), so the 'bad' modulation does not expand or compress as you would expect. When you take the FT of the time domain data, the true modulations transform to the same frequency regardless of step size whereas the bad modulations shift significantly.

The converse test entails leaving the temporal parameters (pulse separations) of the experiment invariant and let the boxcar sample the echo amplitude for the period of a given experiment. A variation of this type of experiment is used to

determine the characteristic frequency spectrum of a boxcar apparatus,¹ but that's a story for another column.

Assuming that I've identified my renegade peak and that it is of sufficient magnitude to be annoying in the FT-spectrum I want to publish, I have two options. I can filter it out mathematically, which has the associated problem that I may filter out something I actually want nearby (with some of the low frequency quadrupole couplings there sometimes

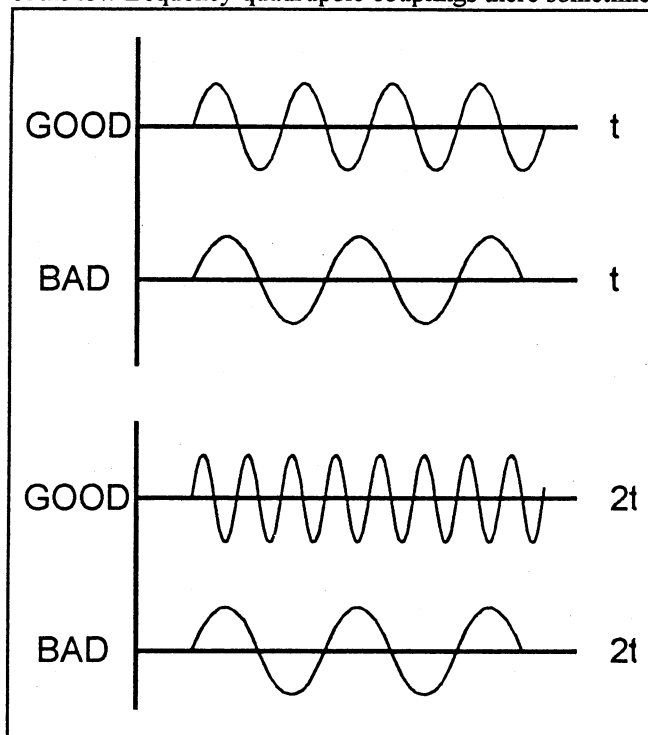


Figure 4: Scaling of the wanted data by changing the incremental step size (here shown as a factor of 2) of the time series while collecting the data at the same rate. Artifacts do not scale accordingly.

gets to be a problem because of overlap, harmonics, etc.). If my spin system provides sufficiently long (desired) oscillations, say, out to 15 - 20 μs , I use a step size long enough to send the spurious modulation below 50 kHz in the FT-spectrum (you have to be careful about undersampling the true nuclear modulations, however. An alternative that seems to work much better entails reprogramming my data acquisition procedure. Rather than collect an entire data set sequentially (i.e. 1000 time points, each an average of

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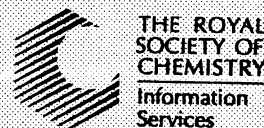
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several hundred), I collect a full 1000 point trace with fewer averages per point (20 - 50). I then cycle back to the starting point and repeat the data collection again. This captures the bad modulation waveform before it completes one period. As successive scans are added, I sum period waveforms that are out of phase (destructive interference); the true modulation is always in phase and adds constructively (timing jitter on our spectrometer is on the order of several hundred picoseconds and does not significantly lead to destructive phase shifts when data are collected in this way provided the step size is >5 ns).

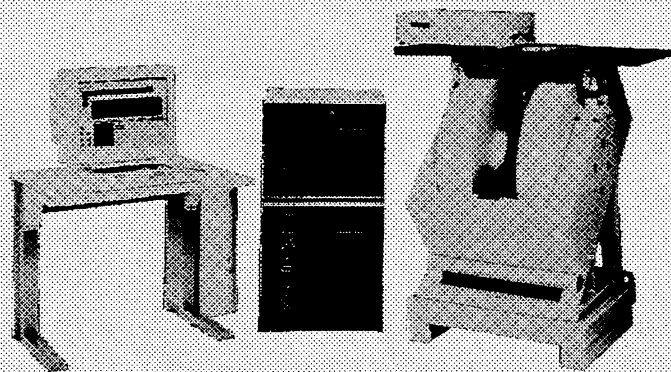
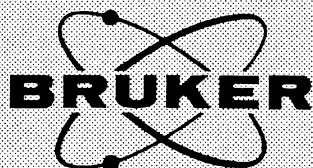
Lastly, there are instrumental methods for making a receiver phase-invariant. I am gradually wading into the radar literature and finding discussions of signal processing topics that are relevant to electron spin echo. For example, one problem common to radar and ESE is the falling edge of the TWT pulse, which introduces phase noise.^{2,3} There are phase-invariant receivers⁴ that are built on a basis of quadrature detection (Figure 4), but I have not yet begun experiments with such a configuration.

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LITERATURE NOTE: The March issue of the *Review of Scientific Instruments* features an article entitled "Magnetic Resonance Spectral Reconstruction using Frequency Shifted and Summed Fourier Transform Processing" (*RSI* 66, p2453-64), by W.G. Clark, M.E. Hanson, F. Lefloch, and P. Ségransan. The article describes the theory of signal processing echo-detected methods of recording inhomogeneously broadened spectra (i.e. field swept EPR using the echo intensity as the measurement criterion). The value of this article lies in their analysis of the method and the demonstration of an alternative technique that eliminates artifacts from small tuning errors (phase shifts).

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up his antenna. It's called an RF Analyst and can be used to measure capacitance, inductance, impedance, and SWR over an operating frequency of 1 - 37 MHz. A recent issue of the ARRL magazine *QST* (May 1995) describes the device and compares test results against an HP8357 network-analyzer. It seems to work well enough for matching ENDOR coils. The cost is \$130, and it is available from Autek Research, P.O. Box 8772, Maderia Beach, FL 33738. 813-886-9515

MORE ON GASSY KLYSTRONS - Clarence Arnow of Micro-Now sent me a FAX message with another way to test for gassy klystrons. One test is the magnitude of the heater resistance, which should be less than 2 ohms. The second is a current measurement criterion of the tube when it is powered up. With the voltage in the normal operating mode, measure the current between the reflector and the reflector supply; the current should be less than 1-2 μ A.

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My magnet has developed a water leak. I would appreciate it if I could receive information on:

1. How to repair it, if possible;
2. Is there any one who has a spare magnet to sell or give away to replace the one I have. We have a very limited budget, but our research is temporarily stopped because of the leak.

With thanks in advance, Sushil K. Misra, Professor of Physics, Concordia University, 1455 de Maisonneuve Boulevard West, Montreal, Quebec H3G 1M8, Canada
Phone: 514-848-3278, Fax: 514-848-2828; E-mail: skmisra@vax2.concordia.ca.

Dear Professor Misra,

We have been there and done that. We have repaired the leaks in our Varian 12 inch magnet ourselves (twice) and it is still working.



Medical Advances
CONTRIBUTOR to the International EPR Society

*"Supplier of Loop Gap Resonator EPR Probes
and EPR Spectrometer Sub-systems"*

Contact: Medical Advances, Inc.
10437 Innovation Drive
Milwaukee, WI 53226 USA
Phone/Fax: 414-258-3808/414-258-4931
email: stevens@medadv.com

We removed the pole faces carefully by building a support under them so that when free we could roll them out without damage. We had to do this to get enough space to be able to remove the magnet coil. They are heavy and should not be dropped. As a precaution we marked the orientation.

After undoing all the cables and water supply pipes and the positioning stop at the front we slid the coil out and onto a support between the magnet faces. Then using our workshop mobile crane we lifted the coil out and onto a trolley for transport to the workshop.

The leak will be at the yoke face of the coil (if it is the same as ours). Using an angle grinder we carefully cut the edge of the plastic case and then removed all of the plastic from the back face which covers the copper cooling plate. Once the copper plate was visible it was easy to see where the corrosion had taken place. We used a big soldering iron and some extra flame heating to solder up the holes. The first time we did it we did not check to see if there were any other weak spots. We had to do it again 18 months later. I suggest that you test for leaks again before putting the coil back in place and cover any possible weak spots. It is now 4 years since the last episode.

We used a disc of 4mm PVC sheet to replace the old casing and used heavy pvc tape to fix it to the rest of the coil. It does not look quite as good as new but it works.

We found that by taking time to make the supports at just the right heights it speed up the removal and reinstallation. The whole operation took about a day.

If you have any other questions please contact me: Rod Claridge, Dept Chemistry, Univ. Canterbury, Christchurch, New Zealand; ☎: 64-3-3642-442; FAX: 64-3-3642-110; E-mail: r.claridge@chem.canterbury.ac.nz.

Dear Prof. Misra :

I would like to share with you my modest experience on solving a similar problem. I had another problem with my 30 years old Varian 12 inch magnet. When I got it, I found, that one of the cooling coils is practically sealed and I have no possibility to work at high field (>8 kG) for a long time. Trying to improve the situation, I studied step by step all magnet cooling system and made the following conclusions:

1. The cooling system consists of two (input and output) metal tubes. Every current coil (left and right) has two copper water circuits connected in parallel to input and output coils by rubber tubes. If you have a leak in this part of the system, it can be repaired very fast and easy by a technician or even by yourself.
2. Practically, there is no possibility to repair something inside the closed coil without serious damage for its covering and coil itself. But ! You can try (by consequent disconnecting of rubber tubes from inlet tube) to find out

in which of your four water circuits there is a leak and then disconnect this tube from all water. In principle, you will have the possibility for normal EPR work. For example, after understanding that our closed tube is damaged mechanically inside the coil, I am working with one circuit closed for a year without any problem for all X-band measurements with very modest cooling of inlet water. When I need to work at high fields (for low field pulsed NMR) I have to increase water flow or to improve cooling. In this case it is possible to work at 1.2 T for some hours before the temperature sensor will switch the magnet off. Maybe these experiences will help to save you time and money.

I understand your case may be more complicated than variants which I have analyzed. In this case, please, sorry for wasting your time. Dr. Alexander I. Shames, Department of Physics, Ben Gurion University of the Negev, P.O.B. 653, Beer-Sheva, Israel; ☎: 972-7-472458; FAX: 972-7-472903; E-mail: sham@bgumail.bgu.ac.il.

COMPANY PROFILES

OKLAHOMA MEDICAL RESEARCH FOUNDATION SPIN TRAP SOURCE

The method of spin trapping utilizing EPR detection has suffered severe problems at the hands of commercial sources of spin traps. This is because the organic synthetics industry have not been cognizant of the need for "EPR-pure" grade materials for the spin trapping needs of the user community. Spin traps prepared at 90-95% purity can potentially introduce a large artifact into the experiment either through the presence of an impurity which is more reactive towards radicals than the spin trap, or via a huge background EPR signal. DMPO as an example has been offered to the purchaser with these problems without apology.

In order to provide EPR-pure spin traps for the free radical practitioners OMRF-STs was organized. Commonly used and newly synthesized spin traps of EPR-pure grade are offered for purchase by OMRF-STs essentially at cost. At this time the synthetic laboratory site is part of the Free Radical Biology and Aging Research Program at the Oklahoma Medical Research Foundation. Dr. Yong-Kang Zhang is the sole employee. Please call or fax for inquiries: ☎: 1-405-271-7950 FAX: 1-405-271-1437.

MEDICAL ADVANCES, INC.

Medical Advances was incorporated in July 1985 as a transfer agent for the engineering and commercialization of university based research. The company was spawned from

the research efforts of the Medical College of Wisconsin, specifically the National Biomedical Electron Spin Resonance Center, which now is called the Biophysics Research Institute. The technology of interest was loop-gap resonators for both EPR and magnetic resonance imaging and spectroscopy RF coiled.

Ten years later Medical Advances employs 48 people, with 20 of these people engaged in the engineering function. On a worldwide basis the company has over 1,500 customers, with most of these customers being MR systems users in medical centers, hospitals and diagnostic imaging centers.

Though the EPR resonator and accessories business for Medical Advances is relatively small in comparison to the larger MR RF coil business position, the company is dedicated to being the innovative supplier of unique products for the EPR community.

Medical Advances will quote on production S-band and X-band loop-gap resonators as well as special order resonators at other microwave frequencies. In addition the company through its affiliation with JAGMAR, the Crocow, Poland based engineering firm, will quote on special order engineered microwave bridges for various types of EPR spectrometers.

HISTORY AND FACTS

Origin:

MR Imaging Coils, called loop-gap resonators, were a development of the Radiation Biophysics Section of the Department of Radiology (now the Biophysics Institute), Medical College of Wisconsin, Milwaukee. The work was based on research conducted by James S. Hyde, Ph.D. and his colleagues at the National Biomedical Electron Spin Resonance Center, also located at the Medical College of Wisconsin.

The initial effort of the design and testing of the local coils was started in 1981 by Hyde and Wojciech Froncisz, Ph.D. and colleagues.

In December 1984 the clinical investigation using the local coils began at the Medical College of Wisconsin on a General Electric 1.5T Signa MR System.

The Medical College of Wisconsin Research Foundation (MCWRF) invited two former General Electric executives to a briefing session on the development of RF local coils for magnetic resonance diagnostic systems. The purpose of the meeting was to explore the possibility of forming a company to take the technology and product prototypes to market.

The Beginning

Medical Advances, Inc. (MAI) was incorporated in July 1985 as a Wisconsin Corporation. Operations commenced in December 1985. The first product was built and sold in January 1986.

Business objectives: (1) Build specialty imaging and spectroscopy coils for MR users, (2) Provide second sourcing to MR manufacturers for "starter kit" coils, (3) Address the laboratory spectroscopy market with innovative designs in ESR probes, (4) Develop supplies and accessories to be used in conjunction with MR and other diagnostic imaging modalities, (5) Be the manufacturing and sales/marketing conduit for university based research in medical and analytical instrument products, (6) Serve as a distribution network for companies desirous of access to the MR market, (7) Provide contract factory service and manufacturing to electro-mechanical manufacturers.

Principals: William (Bill) Zabriskie, Chairman of the Board, and Richard (Rich) Stevens, President.

Current Status:

- A facility with 16,000 sq. ft. was secured by MAI on the grounds of the Milwaukee County Regional Medical Center. The facility is in close proximity to MCW, the site of both the local coil research and the clinical evaluation program. Part of the grounds has been designated the Milwaukee County Research Park and Technology Innovation Center, an urban concept for new and existing companies engaged in the medical technologies.
- MAI's current employment is 48.
- Over 1,500 customers worldwide being served with over 5,000 MR coils or accessories from Medical Advances, Inc.
- MR coil interface achieved with the following MR system manufacturers: General Electric, Siemens, Elscint, Picker, Toshiba/Diasonics.
- ISO-9001 Certified, 1993.

For more information about Medical Advances and its products contact: Richard J. Stevens, Medical Advances, Inc., 10437 Innovation Drive, Milwaukee, Wisconsin 53213, USA; ☎: 1-414-258-3808, ext. 101, FAX: 1-414-258-4931; E-mail: stevens@medadv.com.

CONFERENCE REPORTS

ISMAR95 & EPR WORKSHOP

The ISMAR95 meeting in Sydney, Australia, held from July 16-21, was preceded by an EPR Workshop. Attending one or both meetings were such stalwarts as Jack Freed, James Hyde, and Betty Gaffney. All in all they were marvellous meetings. The workshop included papers by Hal Swartz on *in vivo* EPR and Jack Freed on dynamic imaging of diffusion and FT EPR in the study of membranes, fluids and polymers. Betty Gaffney speculated on the future role

of high frequency EPR in studying the structure and mechanisms of non-heme enzymes and gave us a rundown on her group's studies on lipoxxygenase. On the whole there was much emphasis on advanced techniques. Bruker's Peter Hofer gave a talk on hyperfine spectroscopy by multiple-resonance time-domain EPR and ENDOR techniques in two and three dimensions. I have a copy of the full program on file and will post it on the ISU list server. We have to thank Graeme Hanson of the UQ Mag. Res. Centre and John Pilbrow of Monash Physics for the success of the workshop.

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The ISMAR95 Conference also had much of interest to EPR folk and much to remind us of the commonalities between the two magnetic resonance techniques.

Over all, there was the warm Sydney hospitality and the city turned on its best weather for us -- bright clear Winter days of 16-22 C°.

Cyril Curtain, Monash EPR Group
Clayton, Victoria, Australia 3168

EPR in Living Systems and Condensed Matter

Round Table Discussion

(Reprinted with permission from

"EPR REPORTS from Ljubljana", No. 4, July, 1995)

As a part of the 9th Symposium, "Spectroscopy in Theory and Practice" (Bled, April 10-13, 1995) a Round Table Discussion was organized dedicated to applications of EPR spectroscopy in the research of living systems and condensed matter. The main goal of the organizer was to present the wide variety of research fields, where EPR has proven to be a useful and efficient experimental tool.

Throughout the day, twenty-one lectures and reports were presented by participants from five European Universities. The list of titles is indicative enough of the diversity of theoretical and experimental EPR approaches that were covered in the program:

- *EPR Studies of Charge-Transfer Doped Fullerenes* (invited lecture, P. Cevc, Ljubljana)
- *Evidence for Bifurcated Hydrogen Bonds in KH_2PO_4* (B. Ravkin, Zagreb)
- *EPR Spectra of Copper(II) Complexes with N,N-dialkyl Amino Acids. The Influence of Water Dissolved in Organic Solvents on the Copper(II) Coordination Sphere* (V. Nöthig Laslo, Zagreb)
- *EPR Studies of Trapping of Radiation Energy by Thioanalogs of the Nucleic Acid Bases* (J. Herak, Zagreb)
- *Determination of Spin Hamiltonian for the Hole-Like Centers in Chlorinated Crystals of Nucleic Acid Bases* (K. Sanković, Zagreb)
- *EPR Spectroscopy and Nitroxides* (invited lecture, S. Pečar, Ljubljana)

- *Synthesis of Acyclic Spin-Labeled Analogs of Muramyl-Dipeptide* (M. Sollner, Ljubljana)
- *Electron Paramagnetic Resonance Study of Human Plasma Lipoproteins* (invited lecture, M. Kveder, Zagreb)
- *The Use of EPR Technique as a Tool to Identify the Mitochondrial Site of One Electron-Redox Shuttle to Dioxygen* (invited lecture, H. Nohl, Vienna)
- *Effect of Hypoxia on the Respiration Rate of Mitochondria* (L. Honzak, Ljubljana)
- *Oximetry in Living Cells as Measured by ^{15}N PDT Spin Probe. Effect of the Medium on the EPR Spectrum Line Width* (D. Dolenc, Ljubljana)
- *Oxygen Penetration into a Cylindrical Aqueous Solution Contained in Gas Permeable Teflon Tubing. An per Spin-Probe Presentation* (M. Schara, Ljubljana)
- *Lateral Heterogeneity of Biomembranes. An EPR Study on Erythrocytes and Fibroblasts* (M. Žuvić Butorac, Rijeka)
- *Domain Structuring of Plant Cell Plasma Membranes* (B. Kim, Ljubljana)
- *Structure and Dynamics of Bacteriophage M13 Major Coat Protein in a Membrane Bound Form* (D. Stopar, Ljubljana)
- *Facilitated Diffusion and Band 3-Mediated Anion Transport* (K.F. Schnell, Regensburg)
- *Modifications of Band 3 by Maleimide Spin-Label* (W. Ibel, Regensburg)
- *Determination of the Fluctuations of the Band 3 Anion Channel by NDS-Proxyl* (G. Angerer, Regensburg)
- *Influence of Temperature on the Transport of Liposome Entrapped Substances into the Skin* (P. Verbovšek, Ljubljana)

Abstracts or any other information are available on request.

As a coordinator of the Round Table Discussion and in the name of all participants, I would like to express special thanks to the organizers of the Symposium, to Marjan Veber and Jana Tepina in particular, and to the Spectroscopic Section of the Slovenian Chemical Society for their efficient logistic and financial support in the organization of the meeting.

Jelka Svetek, Ljubljana, Slovenia

BOOKS & PROCEEDINGS

COMPUTER SIMULATIONS IN BIOMEDICINE.
Edited by H. Power (Wessex Inst. Tech.) and R.T. Hart (Tulane Univ.). This book contains the proceedings of the 3rd International Conference on Computers in Biomedicine, which was held in Milan, Italy, June 21-23, 1995. The conference brought together different scientists who work on the applications of computers to simulate biomedical phenomena, as well as those who develop numerical

algorithms to analyze, manage and visualize biomedical data. Contents include:

- Simulation of Physiological Processes
- Computational Fluid Dynamics in Biomedicine
- Orthopedics/Bone Mechanics
- Electro-Magnetic Simulation
- Imaging Processing
- Data Acquisition and Analysis
- Design and Simulation of Artificial Organs and Non-Conventional Therapy

Price US\$255 (Hardback), 668 pages, ISBN: 1562522450; order from Computational Mechanics, Inc., 25 Bridge Street, Billerica, MA 01821, USA; FAX: 1-508-667-7582, ☎: 1-508-667-5841.

NOTICES OF MEETINGS

ASTM SUBCOMMITTEE E10.01, HYATT REGENCY PEACHTREE CENTER, Atlanta, GA, Jan 30-Feb 1, 1996.

The ASTM is the American Society for Testing and Materials, organized in 1898, as a not-for-profit voluntary standards development system. ASTM Headquarters has no technical research or testing facilities; such work is done voluntarily by 34,500 technically qualified ASTM members located throughout the world. Membership in the Society is open to all concerned with the fields in which ASTM is active. Additional information may be obtained from the ASTM, 1916 Race St., Philadelphia, PA 19103; ☎: 1-215-299-5454.

The ASTM Committee E10 on Nuclear Technology and Applications is divided into several subcommittees, of which Subcommittee E10.01 is concerned with Dosimetry for Radiation Protection and is the Subcommittee of interest to EPR Spectroscopists involved in dosimetry and radiation effects on matter. The Subcommittee meets in January and June and has completed 18 internationally recognized standards for radiation dosimetry published in the ASTM's Annual Book of Standards, Section 12, Volume 12.02 Nuclear(II), Solar, and Geothermal Energy.

Standards currently being revised or formulated include "Standard Practice for Use of the Alanine-EPR Dosimetry System" E-1607-94 and "Standard Practice for Blood Irradiation Dosimetry" E 10.01X.

The next meeting will be held at the Hyatt Regency Peachtree Center in Atlanta, GA between Jan. 30 and Feb. 1, 1996. The Chairman of the Subcommittee and the person to contact for more information is Dr. Harry Farrar IV, 18 Flintlock Lane, Bell Canyon, CA 91307-1127, ☎: 1-818-340-1227, FAX: 1-818-340-2132.

THE FOURTEENTH INTERNATIONAL CONFERENCE ON RADICAL IONS, Uppsala, Sweden, July 1-5, 1996.

The Radical Ions conference is a continuation of previous Gordon Conferences 1968-1992 (totally 12) and the

corresponding conference held in Halifax in 1994. Following the traditions the conference will feature invited speakers and poster sessions with time for informal discussions. There will also be space for a number of short oral presentations.

The meeting will take place in the main building of Uppsala University, built in the center of Uppsala in the end of the last century. Uppsala is centrally located in Sweden, with excellent connections both by air (Arlanda airport), by train and by car.

The invited and contributed papers will be published in Acta Chemica Scandinavica as Minireviews, Articles or Short Communications, whichever appropriate, and will be collected into a bound Symposium volume by the organizers. Regular refereeing procedures will be applied.

A significant part of the studies to be presented will involve EPR as a tool. Topics to be covered in the invited talks include:

- Spectroscopy and matrix isolation techniques.
- Radical ions in photochemistry and radiation chemistry
- Synthetic applications of radical ions
- Radical ions on surfaces
- Radical ions in biological systems
- Radical ions in electrochemistry
- Quantum chemical techniques

The registration fee of \$250 for active participants. The cost for a first class hotel, centrally located, is approximately \$70/night, breakfast buffet included, but there are cheaper accommodations in student dormitories that can be arranged. The total number of participants is limited to about 100. Acceptance will be on a first-come, first-served basis. More details are available in a first circular that will be distributed to those interested in attending the conference. To obtain the circular, contact Mari Lofkvist, Secretary, RADICAL IONS 14, Department of Physics, IFM, Linköping University, S-581 83, Linköping, Sweden. For further information about the scientific programme please contact one of the chairmen: Anders Lund, Dept. Physics, IFM, Chemical Physics Laboratory, Linköping Univ., S-581 83, Linköping, Sweden, FAX: 46-13-13-22-85, E-mail: ald@irm.liu.se; Sten Lunell, Dept. Quantum Chemistry, Box 518, Uppsala Univ., S-751 20, Uppsala, Sweden. Or communicate by FAX or E-mail: FAX: 46-18-50-24-02, E-mail: lunell@kvac.uu.se.

NINETEENTH INTERNATIONAL EPR SYMPOSIUM at the 38th Annual Rocky Mountain Conference, Denver, CO, USA, July 21-25, 1996.

For more information contact: Prof. Sandra S. Eaton, Univ. Denver, Dept. Chemistry, Rm. 153 Seely G. Mudd Science Bldg., Denver, CO 80208, USA; ☎: 1-303-871-3102; FAX: 1-303-871-2254; E-mail: seaton@du.edu or Prof. Gareth R. Eaton, Univ. Denver, Dept. Chemistry, Denver, CO 80208, USA; ☎: 1-303-871-2980; FAX: 1-303-871-2254; E-mail: geaton@du.edu.

**FIRST INTERNATIONAL SEMINAR ON
SIMULATION MODELLING IN
BIOENGINEERING (BIOSim 96), Merida,
Venezuela, October 24-25, 1996.**

The objective of this International Seminar is to bring together scientists who are carrying out research on the applications of computers to simulate biomedical problems. The Conference will be held at the Cultural Centre 'Tulio Febres Cordero', Merida. Conference topics will include:

- *Simulation of Physiological Processes*
- *Biomedicine*
- *Electrical and Magnetic Simulation*
- *Imaging Processing*
- *Data Acquisition and Analysis*

Inquiries and abstracts (by December 1, 1995 if possible) should be sent to Sue Owen, Conference Secretariat, BIOSim 96, Wessex Inst. Technology, Ashurst Lodge, Ashurst, Southampton, SO40 7AA, UK; ☎: 44-1703-293223; FAX: 44-1703-292853; E-mail: cmi@uk.ac.rl.ib; Intl. E-mail: cmi@ib.rl.ac.uk.

**POSITIONS WANTED
and
POSITIONS AVAILABLE**

Notice: To save space in this Directory issue, no positions listings are printed. See the previous edition of the Newsletter for such listings.

**EQUIPMENT & SUPPLIES
EXCHANGE**

Notice: To save space for the Directory, repeat Equipment and Supplies Exchange items are suspended for this issue only. Please consult previous issues for such items.

WANTED: EPR CAVITY

The Institute of Mineralogy, University of Marburg, Germany is looking for an EPR cavity for a Varian Model E-110 EPR, Q-band spectrometer. We would like to acquire a used cavity. If you have one available please contact Stefan Hafner, Inst. Mineralogy, Univ. Marburg, 35032 Marburg, Germany; FAX: 49-6421-288919; E-mail: hafner@mail.uni-marburg.de.

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- 2) a E110 Q-band Bridge with cavity

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For more information contact Clarence Arnow, President.
Voice: 708-677-4700 fax:708-677-0394

ANNOUNCEMENTS:

MAILING LISTS FOR SCIENTIFIC MEETINGS

If you are planning a scientific conference, you may contact an officer of the International EPR Society or the IERC (address on front page of this Newsletter) to obtain a list of the 1,300+ Society members for use in issuing invitations. If you would like to have preprinted mailing labels, Martha Moore, who provides secretarial support for the Society, can do this at cost -- approximately \$50.00 (includes cost of labels, postage and, if you wish, a disk copy of the list in ASCII format). Labels for the entire database (3,800+ members and non-members) would cost approximately \$175.00.

*RECENT CHANGES IN PHONE AND FAX
NUMBERS FOR INTERNATIONAL DIALING*

The Netherlands has recently changed many of its city codes. We have tried to make changes for the directory, but if you have difficulty dialing any of the numbers listed for members in the Netherlands, feel free to contact the IERC directly by e-mail (ierc@uiuc.edu) for assistance.

ANNOUNCEMENT

Members: Have you paid your dues? If you are not sure, it will save the Society the expense of mailing late notices if you will take a moment to ascertain the status of your membership according to our records. To do this, please check the lower right hand corner of your mailing label. You will find there four dashes ("-- --"). If only the four dashes "-- --" or "--0--" appear, no dues have been recorded for you for the 1995 year. If dues have been paid, either a numeric value or the letter "R" or "C" (for soft currency countries) will appear, e.g. "--30--". If you don't have your label, please contact the IERC (address on page 1) and we will check to see if dues have been recorded. Your prompt payment of dues will be appreciated! For information on the amount of dues and methods to pay, please see the Appendix.

INTERNATIONAL EPR(ESR) SOCIETY

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APPENDIX

DISTRIBUTION LIST FOR THE EPR NEWSLETTER (TAKEN FROM THE INTERNATIONAL EPR(ESR) SOCIETY, THE EPR NEWSLETTER, AND THE ILLINOIS EPR RESEARCH CENTER DATABASES)

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The following list is provided as a service to the Members of the International EPR(ESR) Society (IES) in the hope that you will find it to be a useful reference. Please note that this list is copyrighted and may not be used in whole or in part for commercial purposes without written permission from the Illinois EPR Research Center or the Editor of the EPR Newsletter.

The information contained in this list includes names of members and non-members of the IES. For each individual who has supplied us with information on his or her main interests, up to five interest codes are included. See the application form at the back of the Newsletter for a list with an interpretation of those codes.

Dr. Peter Gast, University of Leiden, first suggested printing such a list, and he volunteered to produce the final copy in a form suitable for reproduction. We are grateful for his efforts. In the next issue of the newsletter we will print a list sorted by country, which many members have requested.

If you notice errors, including incomplete or out-of-date entries or apparent duplications, please contact us with full details.

For the convenience of Members who wish to pay dues and/or provide updated information and of others who wish to join the IES, a membership registration form is included after the list.

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EPR NEWSLETTER

Volume 7, Number 3

Page 1

Fall/Winter, 1995

- Editor: R. Linn Belford, Urbana, IL (address below).
- Assistant Editor, Becky Gallivan, Urbana, IL (address below).
- Typography: Martha Moore. *This, the official newsletter of the International EPR(ESR) Society, is supported by the Society, by corporate and other donors, and by three EPR/ESR centers:*

National Biomedical ESR Center,

Prof. James S. Hyde, Director, Medical College of Wisconsin, MACC Fund Research Center Building, 8701 Watertown Plank Road, Milwaukee, WI 53226, USA. ☎: 414-456-4008.

FAX: 414-266-8515. E-Mail: cfelix@mis.mcw.edu

WWW: <http://141.106.72.102/BRI-EPR>

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rlbelford@uiuc.edu

† [IERC satellite site for EPR in viable biological systems at Dartmouth College, Hanover, NH; USA.

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

FROM THE EDITOR

Important notice: It hurts me to have to announce this, but our IES President and Treasurer point out that several IES memberships have been allowed to lapse while quite a few of these former members are receiving all the Newsletter issues. Henceforth, both costs and fairness will prevent us from sending any future members' issues to those who have not paid a subscription in the last two years. Anyone who has not paid but wishes to remain an IES member and to receive EPR Newsletters should contact the Treasurer (or a regional treasurer) immediately for reinstatement! (I know, friends, it's easy to forget, but please don't forget it any longer! It's a worthwhile cause, and inexpensive.)

Finally, perhaps you have not been an IES member, but you see this Newsletter and enjoy reading it. In that case, please join the Society! You will find membership registration forms and instructions in many Newsletter issues and in the IES World Wide Web home page: <http://ierc.scs.uiuc.edu/IES.html>

Reminder: The IES Awards Committee begins its work in January to select 1996 awardees, so consideration of additional nominees cannot be guaranteed. But please, as soon as possible, do give the committees your suggestions for 1996 and also, start thinking about nominations for 1997! See *IES Affairs* below for details.

Congratulations: It pleases me greatly to inform my colleagues that Professor John R. Pilbrow, our distinguished colleague, regional treasurer of the IES, and my good friend, has been appointed to a Personal Chair in Physics at Monash University, Melbourne, Australia. The many EPR Newsletter readers who know John will surely join me in congratulating him on this richly-deserved honor.

The Zavoisky Award: In the previous issue, we announced that Professor James S. Hyde was named to receive the 1995 Zavoisky Award. In the *Conference Reports* section of this issue, you will find an account of the symposium and other events that accompanied the ceremonies at which he was given this award.

EPR Newsletter on the World Wide Web: There is now a World Wide Web site for the EPR Newsletter. Its URL address is <http://ierc.scs.uiuc.edu/news.html>

Our intention in creating this Web site is not to publish the Newsletter electronically, but rather (1) to provide auxiliary material like program listings that are not printed in the Newsletter proper, (2) to provide advance information about content of recent and upcoming issues (by listing the Contents), (3) to explain what the Newsletter is and how it can be obtained, and (4) to make auxiliary announcements from the editorial offices. We would very much appreciate your suggestions and comments regarding this site.

R. Linn Belford

◆ **IES AFFAIRS** ◆
**ANNOUNCEMENTS AND
 REPORTS FROM THE INTER-
 NATIONAL EPR SOCIETY**

From the President —

One of the joys of being President of the International Society is to be able to wish all of its members a very happy and successful New Year on behalf of the Committee. This is the last time this particular committee will be able to do this for by this time next year the present Officers will have been replaced by our successors. The changeover will not occur until the beginning of September but elections will have to occur much earlier, of course. Although the Committee intends to suggest names for all the posts, we should welcome any nominations from our members. As we continually remind you, the Society is yours, and it is essential to its well-being that the membership is involved in important decisions such as this. From our point of view, we are determined to remember that we really are an international society and that we must ensure world-wide representation on the executive committee.

We also should like to suggest that we introduce a stagger into the replacement of posts so that continuity is preserved and we do not experience a complete change in personnel at any one time; we have it in mind that the Secretary should continue in office for a further year before he is replaced, and thereafter this post will revert to the normal three year period.

Our Treasurer, David Greenslade, has had to resign from his position earlier than scheduled for reasons entirely beyond his own control. David has been a great servant to the Society, and has been a tower of strength to me personally in the way he has administered our finances and given wise advice. I should like to take this opportunity of thanking him on all our behalf for all the work he has put in. This position is of maximum importance to us and we have

been very fortunate indeed to have David replaced by Prof B. Kalyanoraman. He has been appointed by the President as Acting Treasurer until he can be elected properly when the position has formally to be re-filled in September. I am very grateful to Raman for accepting this post, as I am sure we all are.

It became apparent during David's period that since most of the expenditure of the Society is associated with publication of the Newsletter, and most of the funds arrive in US dollars, then it is inconvenient to have a Treasurer from outside of the US. In Raman's case we are particularly pleased to have him in the same centre as our US regional Treasurer, Chris Felix, where they will form a formidable team. He is already proving a lively new member of the committee and is reminding us how valuable it is to get new blood onto it from time-to-time.

All this implies that the posts for which nominations are needed are those of President and Vice-President. We have some first rate suggestions to make for these, but Hal Swartz, as Chairman of the Nominations Committee, would welcome any further nominations being made to him. We should also consider changes in Council (list provided for reference on p. 25) at the same time, with perhaps one third of its membership changing; again any proposals would be gratefully received by Hal.

Keith McLauchlan

Awards

Important: As previously announced, nominations for all the awards of the IES for the coming year are due January 1, 1996. Nominations arriving after January 1 may be considered for the 1997 or 1998 awards if the 1996 award decisions have been made.

We repeat here the Society's award policies: Awards are not restricted to IES members, but the committees may take membership into account when deciding on the award winners. Agreement has been reached between the British and Russian Groups and ourselves to co-operate in the award of the Bruker and Zavoisky Prizes and our Gold Medal Award each year, with each group invited to make input into the selection of each, but with the final choice left to each group. The area of research interest is to rotate between the groups each year, with the loosely-interpreted categories, chemistry, physics and instrumentation, and biological sciences (including medicine), these are meant to be interpreted liberally and not to be restrictive.

In 1996, the IES Gold Medal award will be in Physics and/or Instrumentation, the Bruker in Chemistry, and the Zavoisky in Biology and/or Biological Sciences. Prof. Larry Berliner, continuing Chairman of the Gold Award committee, will welcome nominations for this.



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Gold Medal: 1996 Gold Medal, recognizing benchmark contributions to EPR spectroscopy in physics and for instrumentation. Nominations to Prof. Larry Berliner.

Silver Medals: One each in the general areas of Chemistry, Physics/Instrumentation, and Biology/Medicine. To propose names, please send your suggestion(s), or preferably full nomination(s), to the appropriate Silver Awards Subcommittee(s): *For Physics and Instrumentation* - Jim Hyde, Chair; John Pilbrow, George Feher, & Jan Stankowski. *For Chemistry* - Bruce Gilbert, Chair; N. Hirota, Jim Bolton & Kev Salikhov. *For Biol./Medicine* - Harold M. Swartz, Chair; Marjeta Sentjurc, Hideo Utsumi & Tadeusz Sarna.

Young Investigator Awards: One Young Investigator award each year; "young" is defined as being under 35 on January 1 of the year the award is made. Send nominations to Prof. Keith McLauchlan.

Affiliation of Regional Societies to the International EPR(ESR) Society

1. Affiliation to the Society can be applied for by any local EPR/ESR society which is already in existence or which is about to be formed.
2. In any affiliation the IES remains the sovereign Society, and the affiliated one is subject to all of its rules and by-laws. It may, if so wished, establish further ones of its own.
3. The object of affiliation is to allow local societies to benefit from being associated with the world-wide EPR/ESR community represented by the IES, and from its contacts, publications, publicity, advertisements, etc.
4. The role of the affiliated society is to extend the influence and availability of the IES throughout the world, and to provide those services most appropriate to the local membership, for example in helping to arrange conferences and summer schools.
5. In accepting affiliated societies the IES is mindful of their possible impact on similar societies already established in the same general area of the world. The IES will not accept any society as an affiliated one which might affect the well-being of these pre-existing affiliated ones, or the interests, including financial interests, of the IES itself.

6. The decision as to whether to apply for affiliation must be made by the local society under whatever rules and regulations it itself has.
7. The local society itself will normally be responsible for the dissemination of information concerning the IES to its members and for facilitating communications of individual members with the IES.
8. To be accepted as an affiliated society, at least one half of the members of the local society should be members of the IES. However, membership of a local society by an individual is not a prerequisite for membership of the IES.
9. Each affiliated society is required to provide a local treasurer responsible for collecting the dues from its members in local currency and transferring the total in a single currency exchange at least once a year to the Treasurer of the International EPR Society.
10. All IES members in developed countries pay the standard membership fee of US\$30 (or its local equivalent) per annum, but the Society will consider proposals for levels of fees from other parts of the world which are deemed reasonable by the local treasurer. Members in a number of countries benefit from this arrangement and receive the full privileges of membership notwithstanding. Any members in local societies benefitting in this way are, however, expected to pay in full if they are able to, and the long-term aim should be for all members to pay the full fee. In the meantime the IES is pleased to accept those members who benefit from membership without being able to pay this.
11. All publicity for conferences etc. arranged locally will be published free of charge in the Newsletter, and the IES will be pleased to allow its name to be used in assisting the organization and funding of such meetings; at present it is unable to offer financial support. The organizers will be able to request information from the database to aid arranging and advertising such meetings.

Fellows of the Society

The IES has created Fellowships to recognise truly outstanding contributions and achievements in electron paramagnetic/spin resonance among these scientists (hopefully, IES members) who are either retired or are close to retirement. (Fellows of 1995: Anatole Abragam, Brebis

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Bleaney, Clyde Hutchison, Aleksandr Prokhorov and Samuel Weissman). The highest international standards are to be applied to the recognition of those worthy of this distinction, and their formal connection with the Society will enhance its own image. Nominations for consideration by the Committee are to be sent in confidence to Keith McLaughlan by January 1, 1996.

THE COMPUTER CORNER

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

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

Reef (Philip D., II) Morse	(reef@xenon.che.ilstu.edu)
Graeme Hanson	(graeme@cmr.uq.oz.au)
Keith Madden	(madden@marconi.rad.nd.edu)
Dick Cammack	(udbc033@hazel.cc.kcl.ac.uk)
Dave Duling	(duling@niehs.nih.gov)

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

Linux Operating System by Keith Madden

The recent release of Microsoft's Windows 95 operating system software, amidst a torrent of world-class hype, has overshadowed almost all other developments in the software world for the last year or so. Of particular interest to the computer-oriented spectroscopist has been the quiet, rapid development of the Linux operating system. Linux is a true 32-bit UNIX work-alike for Intel-based personal computers containing a 386 or better CPU. This OS was developed by volunteer programmers throughout the world, who expanded upon the OS kernel written by Linus Torvalds of Finland while he was a college student. Many of the utilities that give the functionality of UNIX have been ported to the Linux OS through the efforts of the Free Software Foundation (FSF). The result is a full-featured operating system available for free at both the source code and binary executable level via the internet. The OS bears the GNU copyright of the Free Software Foundation, which protects the availability of source code for the user of the software. The advantages of this OS are as follows:

1. The software is free.
2. The software is complete -- the Linux distribution contains not only the system kernel and the system utilities, but also a full set of tools for software development, communications, publishing, and system administration. In particular, an implementation of the X windows system is included so that GUI-based user applications can be developed and run.
3. The software is supported -- there are several Usenet groups dedicated to Linux, dealing with new software announcements, system development progress,

hardware compatibility and installation issues. Most distributions of Linux also contain voluminous amounts of information in the form of HOW-TO notes, and frequently asked question (FAQ) documents.

4. The software can be configured to your precise needs -- since the source code is available, as well as the binary files, one can recompile the OS kernel to eliminate unused device drivers, and to accommodate special circumstances in one's computer hardware.
5. It's great fun.

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Of course, since this software was written by volunteers in their spare time, the current set of applications, although highly functional, lack the sophistication of their commercial counterparts; although the emacs text editor running under X-windows is a great tool, no one will mistake it for Microsoft Word for Windows 6.0 -- but the price is right, and you probably can get support more quickly, with less aggravation, for GNU emacs.

The first issue in starting with Linux is to describe how the operating system is packaged. The Linux kernel itself provides enough software to yield a command-line prompt, but little else. The functionality of the OS is derived mainly through the utilities bundled together with the kernel. Since the kernel is publicly available for free, a number of people have packaged the kernel with their favorite utilities and an installation program to form a distribution set, usually referred to as a distribution. The distribution that I have had the most experience with is Slackware, developed by Patrick Volkerding. This is a slick version of Linux, with good tools included, and a very good installation program.

So how does one get this software and begin to play with it? There are three answers to that question, depending on your resources, and your tolerance for pain. For the least out-of-pocket expense, one can download the software via the internet. Point your favorite internet browser towards fip://sunsite.unc.edu/pub/Linux/distributions/slackware/ -- this is the home of the Slackware distribution. If you examine README???.TXT and INSTALL.TXT you'll get information on how to download and install Linux.

The second method is to buy one of the recently published books about Linux. These almost always include a CD-ROM containing a distribution of Linux. My favorite is Linux Configuration and Installation, by Volkerding, Reichard, and Johnson, MIS Press, New York, 1995. This book is about setting up and using Linux, so that the ambiguities that are not resolved by merely reading the HOW-TO and FAQ documents can usually be resolved by perusing the clear prose of Volkerding et al.

Finally, one can just buy a commercial distribution of Linux, with added commercial goodies. The Caldera Network Desktop is such a product -- for details point your web browser toward <http://www.caldera.com> for information and pricing.

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Next time we'll talk a bit about the installation of Linux, and the joys of getting up and running.

A Contribution from Joshua Telser

I would like to let people know about an EPR/ENDOR simulation program I have written (in FORTRAN) which is available to anyone interested.

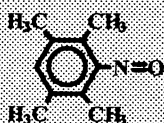
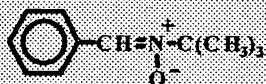
The program is called DDPOW. It used matrix diagonalization for a system of one electronic spin ($S \leq 5/2$) and one nuclear spin ($I \leq 7/2$). EISPACK routines are used to calculate the eigenvalues and eigenvectors to give the resonant transition frequencies and probabilities for EPR or NMR (ENDOR) transitions.

The igloo method is used to generate a powder pattern. The program runs on a PC (Microsoft FORTRAN 4 or 5) or on a mini/mainframe computer (F77). It is rather slow, except for simple systems, but fast if you just calculate the principal transitions (single crystal values, g_x, y, z).

There are two other programs available, DDPOWJ and DDPOWJH; the former is for a system of two electronic spins with exchange (J) coupling to give EPR spectra, and the latter is for the case which has two S's and two I's (i.e., a combination of DDPOWH & DDPOWJ). The versatility of DDPOWJH does result in slower execution, however.

I don't think there are any serious flaws in the program by now, but would look forward to comments from any interested users. I can be contacted as follows:

Joshua Telser, Roosevelt University, 430 S. Michigan Ave., Chicago, IL 60605, USA; VOICE: (312)341-3687; FAX: (312)341-3680; E-mail: telser@chem.nwu.edu.

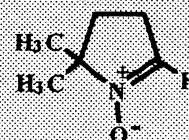
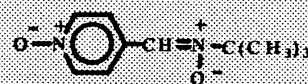


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The IERC (ierc.scs.uiuc.edu) and Illinois State University (xenon.che.ilstu.edu), in cooperation, maintain anonymous ftp servers which include vendor demonstration programs (xenon), public domain software (ierc), and Rich Cammack's software data base.

More computer stuff in this issue

If you read the "Tips & Techniques" column below, you will find an account by C.P. Lee of outfitting an older EPR spectrometer with computer capability.

EPR SPECIALIST VIGNETTES

Edited by
Arthur Schweiger

COHERENCE TRANSFER ECHOES IN EPR

by Alessandro Ponti

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1. Introduction

Coherence is one of the most important concepts in pulsed magnetic resonance. Coherence is formally defined as any (non-zero) off-diagonal element of the density operator σ which describes the spin system, when σ is expressed as a matrix in the eigenbasis of the system's Hamiltonian and is averaged over a statistical ensemble of systems. The diagonal elements of the above defined matrix representation of σ are the populations of the spin states.

Coherence is closely linked to transitions. Both coherence and transitions connect two states of the spin system: for instance, EPR transitions correspond to coherence between states with $\Delta m_S = \pm 1$ and $\Delta m_I = 0$. We can then classify coherence as to the associated transitions and say that EPR transitions correspond to *single-quantum electron coherence*. It should be mentioned that observable magnetization, and then observable magnetic-dipole transitions, is proportional to single-quantum coherence. Zero- and multi-quantum coherence cannot be observed directly.

A coherent system evolves in time since it is not in an eigenstate of the Hamiltonian. Any single coherence evolves in time with a frequency equal to the frequency of the associated transition:

$$\sigma_{ij} \xrightarrow{\text{evolution for time } t} \sigma_{ij} \exp(-i \omega_{ij} t)$$

In contrast to NMR, many pulsed EPR experiments rely on the observation of a *spin echo*¹, a phenomenon which results from the dephasing (defocussing) and subsequent rephasing (refocussing) of coherence. The presence of an inhomogeneous term in the Hamiltonian is essential since homogeneous dephasing (T_2 mechanisms) is random in nature and cannot be refocused. Of course, it is also essential that we know how to rephase coherence.

2. Regular echoes and coherence-transfer echoes

In a "regular" echo, coherence dephases and rephases on the very same transition. For instance, a regular echo occurs when the primary echo sequence $\pi/2-\tau-\pi-\tau$ is applied to a system consisting of isolated $S=1/2$ spins ruled by an inhomogeneous electron Zeeman interaction $H_0 = \Omega_S S_z$ (Ω_S is the offset from the microwave frequency). In this two-level system there are two transitions $\Delta m_S = +1$ and $\Delta m_S = -1$ which correspond to electron coherences σ_{12} and σ_{21} . Their evolution frequencies are $+\Omega_S$ and $-\Omega_S$, respectively. In Figure 1 the phase accumulated during the primary echo sequence is shown for several spin packets. The echo occurs when all of the electron coherences have the same phase.

In a coherence-transfer echo (CTE), dephased coherence is transferred to *another* transition before refocussing. The process can be formally described as follows:

$$\sigma_{ij} \xrightarrow{\text{1st evo}} \sigma_{ij} \exp(-i \omega_{ij} t_1) \xrightarrow{\{ij \rightarrow kl, \text{2nd evo}\}} C \sigma_{kl} \exp[-i(\omega_{ij} t_1 + \omega_{kl} t_2)]$$

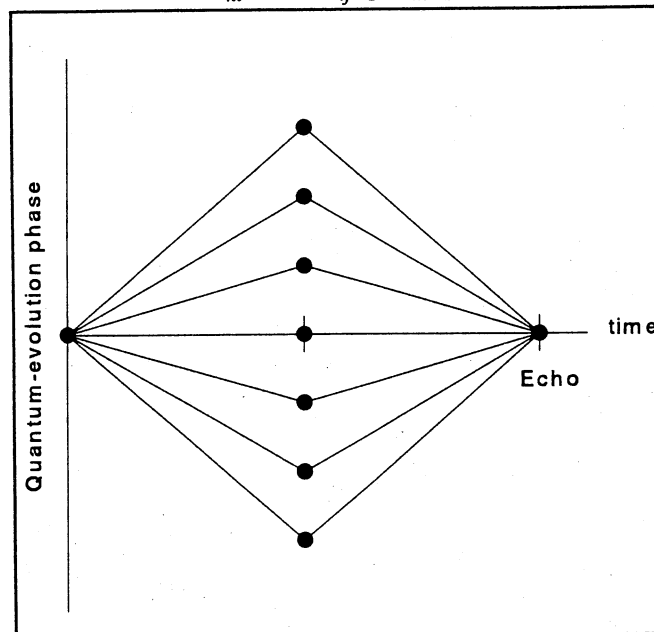


Figure 1. Quantum evolution phase accumulated by the electron coherences in different spin packets during a two-pulse echo experiment performed on a collection of isolated $S=1/2$ spins undergoing inhomogeneous electron Zeeman interaction. The dots indicate the phase at time 0, τ , 2τ .

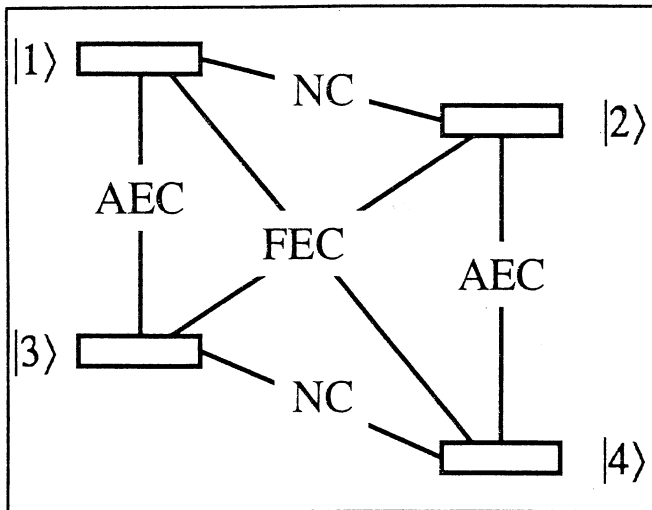


Figure 2. Four-level diagram of the $S=1/2, I=1/2$ model spin system.

A CTE is formed whenever the phase factor $\omega_{ij}t_1 + \omega_{kl}t_2$ is the same for any coherence and the coherence-transfer amplitude C is not zero. In the "regular" two-pulse echo discussed above, $\omega_{ij} = -\omega_{kl}$ and the echo occurs at $t_2 = t_1$. CTEs arising from a transfer of multiple-quantum coherence to observable single-quantum coherence have been demonstrated in NMR². There $\omega_{kl} = -\omega_{ij}/n$ and the echo occurs at $t_2 = nt_1$. The delay is due to the different sensitivity of multiple-quantum and single-quantum coherence to the Zeeman inhomogeneity.

An interesting feature arises when the electron coherences are not completely refocussed, e. g., when an anisotropic hyperfine coupling is present. Assume that $\omega_{ij} = \Omega + \omega_1$ and $\omega_{kl} = -\Omega + \omega_2$, where Ω is the electron-Zeeman part of the evolution frequency. A CTE still occurs at $t_1 = t_2$, but the echo is shifted from the phase it would have if $\omega_{ij} = -\omega_{kl}$. The remaining phase factor amounts to $\exp[-i(\omega_1 t_1 + \omega_2 t_2)]$. The echo is then labelled by the evolution frequencies *before and after* the transfer.

3. Electron coherence-transfer echoes

Among pulsed EPR techniques, two-pulse electron-spin-echo envelope modulation³ (ESEEM) is one of the most widely applied. In this section we show that the modulation of the two-pulse echo arises from the superposition of regular electron spin echoes and phase-shifted electron coherence-transfer echoes⁴.

We consider a simple model system consisting of an electron spin $S=1/2$ and a nuclear spin $I=1/2$ coupled by anisotropic hyperfine interaction, described by the high-field rotating-frame Hamiltonian

$$H_0 = \Omega_S S_z + \omega_I I_z + A S_z I_z + B S_z I_x$$

where ω_I is the nuclear Larmor frequency and A and B are the secular and pseudosecular part of the hyperfine interaction. For the moment we assume that only the electron Zeeman term is inhomogeneous (e. g. a single crystal with a distribution of g -values). The four eigenvalues of H_0 are

$E_1 = (\Omega_S + \omega_\alpha)/2$, $E_2 = (\Omega_S - \omega_\alpha)/2$, $E_3 = (-\Omega_S + \omega_\beta)/2$, $E_4 = (-\Omega_S - \omega_\beta)/2$ where ω_α and ω_β are the nuclear transition frequencies in the $m_S = +1/2$ and in the $m_S = -1/2$ manifold. In the weak-coupling limit the eigenstate correspondence is $|1\rangle = |\alpha\alpha\rangle$, $|2\rangle = |\alpha\beta\rangle$, $|3\rangle = |\beta\alpha\rangle$, $|4\rangle = |\beta\beta\rangle$. The four-level system is pictured in Figure 2. The density operator is represented by a 4×4 matrix with four allowed electron coherences (AEC: $\sigma_{13}, \sigma_{24}, \sigma_{31}, \sigma_{42}$), four forbidden electron coherences (FEC: $\sigma_{14}, \sigma_{23}, \sigma_{41}, \sigma_{32}$) and four nuclear coherences (NC: $\sigma_{12}, \sigma_{34}, \sigma_{21}, \sigma_{43}$). The evolution frequency of each coherence σ_{ij} is $\omega_{ij} = E_i - E_j$.

Because of the anisotropy of the hyperfine interaction, the first pulse excites both AEC and FEC. We focus our attention on the AEC σ_{13} and follow its evolution throughout the experiment (Figure 3). After the first evolution period it has accumulated an inhomogeneous phase factor $\exp(-i\omega_{13}\tau) = \exp\{-i[\Omega_S + (\omega_\alpha - \omega_\beta)/2]\tau\}$. The π pulse, needed to refocus the EC, transfers σ_{13} to allowed and forbidden ECs, i.e., to $\sigma_{31}, \sigma_{42}, \sigma_{32}, \sigma_{41}$, all of which retain the phase factor $\exp(-i\omega_{13}\tau)$. After another evolution period of duration τ , the inhomogeneous phase factor is cancelled and four echoes occur. The $13 \rightarrow 31$ pathway does not involve coherence transfer and its echo is not phase-shifted since $\omega_{31} = -\omega_{13}$ by definition. This "regular" echo contributes to the unmodulated part of the total echo amplitude. The other transfer to an AEC ($13 \rightarrow 42$) yields a CTE phase shifted by $\exp[-i(\omega_{13} + \omega_{42})\tau] = \exp[-i(\omega_\alpha - \omega_\beta)\tau]$. The two transfers to FEC, ($13 \rightarrow 32$) and ($13 \rightarrow 41$), correspond to CTEs phase shifted by $\exp(-i\omega_\alpha\tau)$ and $\exp[-i(\omega_\beta)\tau]$, respectively. The echo envelope then

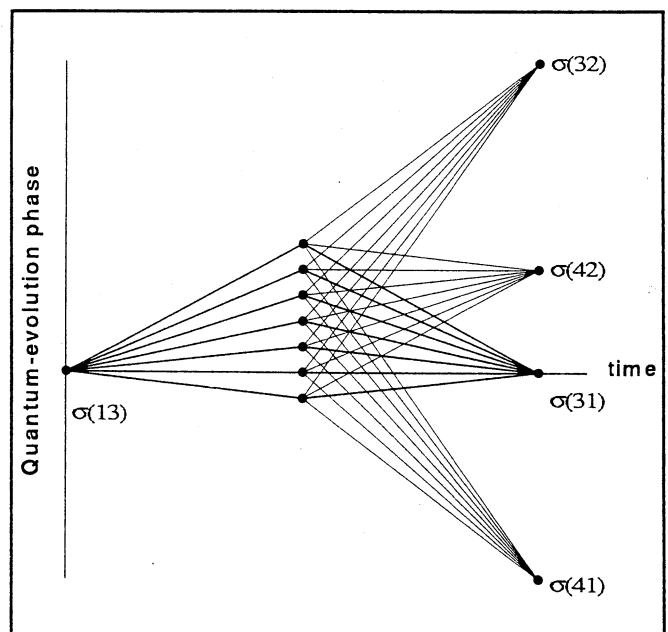


Figure 3. Quantum-evolution phase accumulated by the allowed electron coherence σ_{13} during a 2-pulse ESEEM experiment. The dots indicate the phase at time 0, τ , 2τ . At time τ , the AEC in each spin packet is transferred to four different ECs. Then, four echoes are formed at time 2τ with different phases.

contains contributions whose amplitudes are modulated with the frequencies $\omega_\alpha - \omega_\beta$, ω_α , and ω_β .

The total echo amplitude is the sum of all possible transfers from the eight AEC and FEC excited by the first microwave pulse. Since each EC is transferred to four other ECs, we have a total of $8 \times 4 = 32$ different contributions. For the sake of clarity, Figure 4 shows only the homogeneous part of the phase accumulated by all coherences during the experiment. Out of these 32 echoes, 8 are regular echoes and 24 are CTEs. Out of the 24 CTEs, 8 are AEC \rightarrow AEC and FEC \rightarrow FEC CTEs which are modulated by the nuclear combination frequencies $\omega_\alpha - \omega_\beta$ and $\omega_\alpha + \omega_\beta$, respectively, whereas the remaining 16 CTEs arise from AEC \rightarrow FEC and FEC \rightarrow AEC transfers and are therefore modulated with the nuclear fundamental transition frequencies ω_α and ω_β . The relative weight of the echo modulations can be obtained by a full density-operator description of the two-pulse ESEEM experiment, but our simple argument indicates that the ω_α and ω_β modulations are twice as deep as the $\omega_\alpha + \omega_\beta$ and $\omega_\alpha - \omega_\beta$ modulations.

For any ($ij \rightarrow kl$) transfer there is a ($lk \rightarrow ji$) transfer which has the same efficiency and results in a final phase factor $\exp[-i(\omega_{lk} t_1 + \omega_{ji} t_2)] = \exp\{-i[-(\omega_{kl} t_1 + \omega_{ij} t_2)]\}$. Then, at $t_1 = t_2$, all CTEs occur in pairs symmetrically phase-shifted with respect to the unmodulated echo (Figure 4). Hence their sum is in phase with the unmodulated echo and proportional to the cosine of the phase angle.

If we perform two-pulse ESEEM on a disordered system, also the hyperfine interaction is inhomogeneous. The CTEs interfere destructively with each other and the echo modulation decays quickly, often faster than the echo itself. Since just after a pulse the spectrometer is "blind", the first

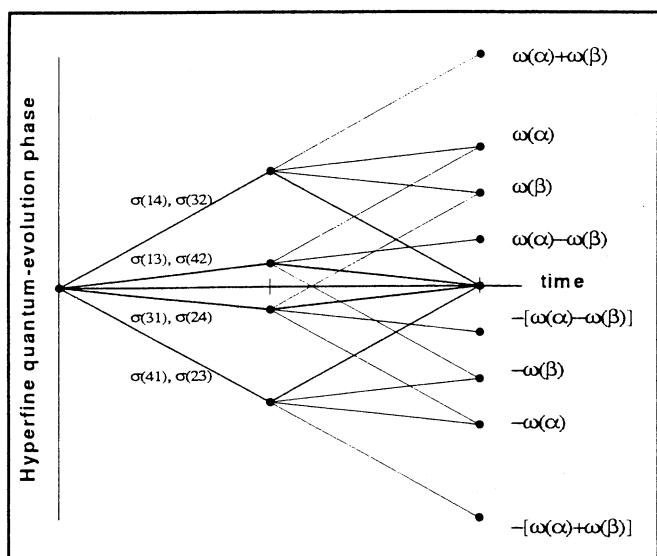


Figure 4. Hyperfine quantum-evolution phase accumulated by the electron coherences during a 2-pulse ESEEM experiment performed on a single-crystal sample. The phase of electron CTEs at time 2τ is reported. The number of CTEs with a given phase is proportional to the number of lines ending in each dot.

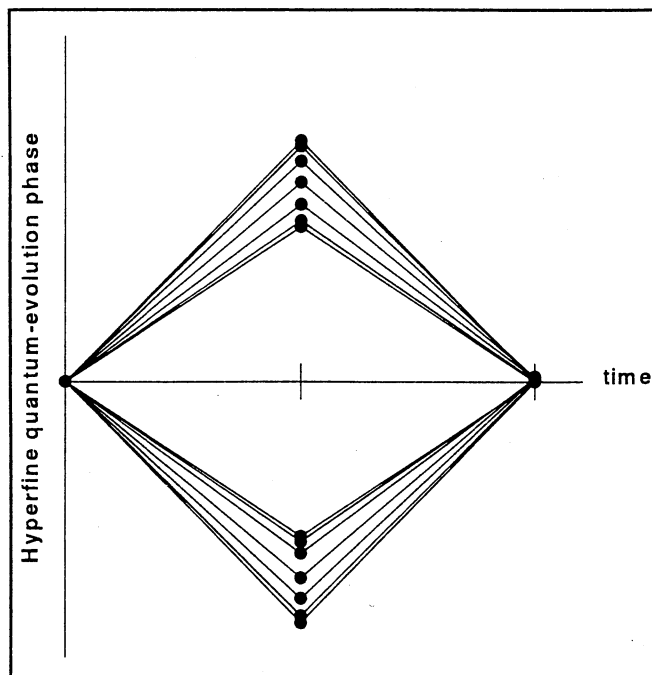


Figure 5. Hyperfine quantum-evolution phase accumulated by the nuclear coherences during the $t_1 - \pi - t_2$ sub-sequence of a four-pulse ESEEM experiment performed on a disordered sample. The lines represent spin systems with axial hyperfine coupling oriented at $0^\circ, 15^\circ, 30^\circ, 45^\circ, 60^\circ, 75^\circ, 90^\circ$ with respect to the external field. Note the incomplete refocussing of the NCs at $t_1 = t_2$.

part of the modulation cannot be observed. This is a serious problem. A very broad line could be completely missed and the loss of information causes distortions and artifacts in the Fourier-transformed spectrum. Many proposals have been made to avoid the dead-time problem and one of them is described in the next section.

4. Nuclear coherence-transfer echoes

The three-pulse stimulated ESEEM is based on the pulse sequence $\pi/2 - \tau - \pi/2 - T - \pi/2 - \tau$. The first pulse excites EC which dephases during τ and is transferred to NC by the second pulse. The individual NCs evolve during T thus accumulating a phase factor $\exp(-i \omega_\alpha T)$ or $\exp(-i \omega_\beta T)$. The last pulse transfers the labelled NC back to EC which refocusses during the last evolution period. The stimulated echo modulation mirrors the NC evolution. We still have to cope with the dead-time problem. The solution is to refocus the NCs (and then the echo modulation) by a nuclear coherence-transfer echo (NCTE). This is accomplished by applying during the evolution of the NCs a microwave π pulse which inverts the electron spin and, consequently, the hyperfine field at the nuclei. This amounts to a transfer of the NCs from one m_S manifold to the other one.

All of the four-pulse ESEEM experiments proposed up to now (HYSCORE⁵, Combination-peak⁶ and DEFENCE⁷) are based on the sequence $\pi/2 - \tau - \pi/2 - t_1 - \pi - t_2 - \pi/2 - \tau$ -echo. Any of them involves NCTEs when performed on disordered systems. The formation of a

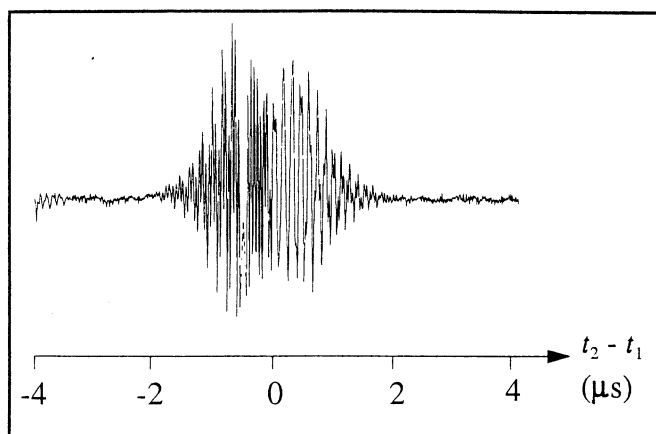


Figure 6. Nuclear coherence-transfer echo modulation recorded in a DEFENCE experiment performed on a powder sample of bis(η^6 -benzene)vanadium(0) diluted into ferrocene.

“regular” NC echo in disordered systems by microwave pulses only has been recently demonstrated⁸.

We focus now our attention on the t_1 - π - t_2 sub-sequence during which NC evolves. At the beginning all possible NCs (σ_{12} , σ_{34} , σ_{21} , σ_{43}) are non-zero but, as before, we follow the destiny of a particular NC. σ_{12} has accumulated a phase factor $\exp(-i\omega_\alpha t_1)$ at the end of the t_1 evolution period. The π pulse transfers σ_{12} to σ_{33} , σ_{34} , σ_{43} and σ_{44} but only the (12 \rightarrow 34) and the (12 \rightarrow 43) transfers can yield a NCTE. After the second evolution period, we have NCs with a phase factor $\exp[-i(\omega_\alpha t_1 - \omega_\beta t_2)]$ and $\exp[-i(\omega_\alpha t_1 + \omega_\beta t_2)]$. It can be easily shown that either the former or the latter phase factor is nearly homogeneous, except when $A, B = \omega_I$ (the so-called matching region). The same argument can be applied to the three remaining NCs. Figure 5 shows the evolution phase accumulated by NC during the t_1 - π - t_2 part of a four-pulse ESEEM experiment performed on a system with a weak axial hyperfine interaction. For the sake of clarity the inhomogeneous electron Zeeman and the homogeneous nuclear Zeeman contributions are neglected. The abrupt change in phase accumulation is the effect of the NC transfer. It can be seen that the refocussing is not complete. Perfect rephasing is hampered by the pseudosecular part of the hyperfine interaction.

The NCTE is observed as amplitude modulation of the four-pulse electron spin echo. In contrast to stimulated ESEEM, the NC are not in phase at the (unobservable) beginning of the experiment (i. e., when $t_2=0$) but at $t_2=t_1$, where t_1 can be chosen at will but shorter than the nuclear T_2 . This allows one to delay the NCTE until the spectrometer has recovered and to record the entire modulation. Thus the shortcomings that arise from the incomplete knowledge of the echo modulation are avoided. In Figure 6 is reported a real NCTE observed in a DEFENCE experiment on a powder sample of bis(η^6 -benzene)vanadium(0) diluted into ferrocene.

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Building The Perfect Beast

Chris Bender

NIH Biotechnology Resource for Pulsed EPR

THE CONCEPTS OF VSWR AND INSERTION LOSS

In the course of spectrometer design and construction, one encounters the terms VSWR and insertion loss when specifying components. VSWR represents Voltage Standing Wave Ratio, and it is a measure of mismatch between a device and the transmission line that provides the input power to that device. Insertion loss is simply the fraction of the power (expressed in decibels) that is lost to reflections or dissipation.

There are a variety of ways in which VSWR can be described, but I am basing this note on a chapter by Anthony Giordano in the Polytechnic Institute of Brooklyn's "Handbook of Microwave Measurements". The advantage of this approach is that the model is mechanical and therefore intuitive.

The starting point of such a discussion is the traveling wave, for example, waves generated by a steady drip of a faucet in an infinitely large bathtub. At some radial distance from the source one could measure the time dependent depth of the water in the bathtub: $D(t) = D_0 + D_1 \sin(\Omega t - \beta r + \Phi)$, where D_0 is the water's depth when the water's surface is placid, Ω is the frequency of the wave, β is a phase constant of the medium, and Φ is an arbitrary phase factor. The important point here is that the waveforms $D(t)$ and $D(r)$ would appear identical. If you stuck a stick in the tank and measured the depth by the level on the stick that was wet, you would find that no matter where you put the stick relative to the source of the waves, the portion of the stick that was wet is the same. This is a property of traveling waves, and the analog of this stick in microwave measurements is the electrical probe (wire pushed in through the wall of a waveguide) connected to a rectifying crystal that puts out a current response to the amplitude of a high frequency signal.

Most of us have splashed around in a wave trough or ripple tank during elementary physics, so much of the following material should be familiar. In a finite system such as a wave trough, one can reproduce the properties of a traveling wave if the tank's boundaries happen to be perfect absorbers of the incident wave. For water waves, this perfect absorber would correspond to a gently sloping 'shoreline'. There is no reflection of the incident wave back into the tank, and all the energy of the wave is transferred to the boundary.

The other extreme is obviously a boundary that completely reflects the incident wave. Stationary waves are set up in such a system, and one would find that the stick (or electrical probe) would register different depths as a function of r . The waveforms $D(t)$ and $D(r)$ do not look the same. The function $D(r)$ is characterized by peaks and troughs, and the troughs appear at $n\lambda/2$.

It should be apparent that the two scenarios that I have described are analogous to loads on a transmission line. Perfectly absorbing and reflecting boundaries in the ripple tank correspond to perfect match and mismatch on an electrical line, respectively. Practical examples of both types of transmission line terminations can be fabricated by closing off the end of a rectangular waveguide. The matched load would simply have a tapered piece of absorbing material (e.g. polyiron, see Poole's text).

One can represent the distinction between matched and unmatched loads graphically, and again the wet stick model

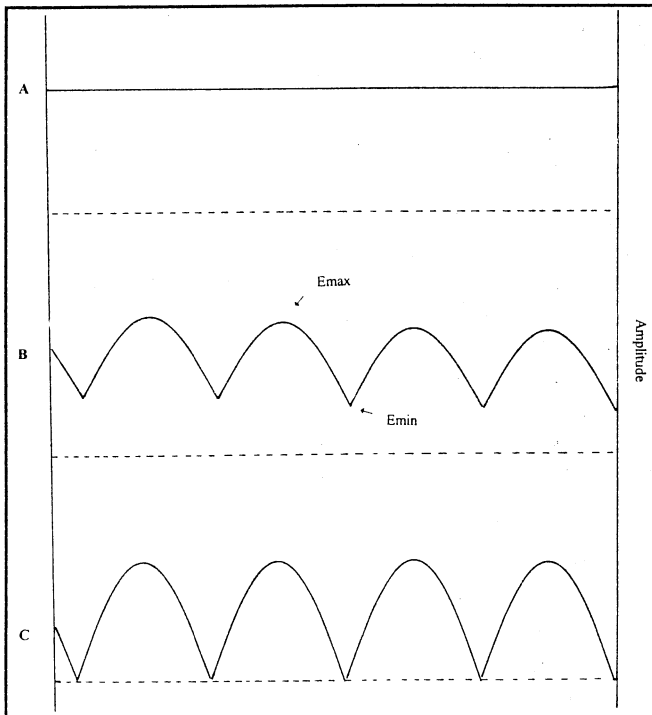


Figure 1. Electric field intensity (analogous to D in the text) as a function of position in a transmission line. A) Travelling wave (no spatial variation); B) Stationary wave, partial reflection; C) Stationary wave, full reflection. All drawn to scale - dashed line is $|E| = 0$.

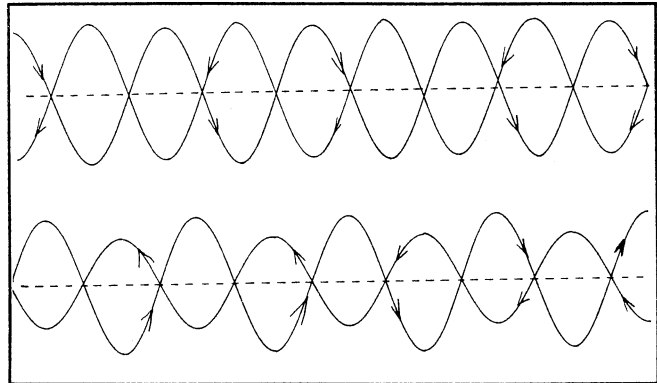


Figure 2. Incident and reflected waveforms in a terminated transmission line. Incident wave moving left to right. Top panel is shorted (100% reflected) line, 180° out of phase reflection. Boundary condition (short at terminus) forces $|E| = 0$ at terminus, hence the $\lambda/2$ relation. Bottom panel is a partial reflection waveform; boundary condition lifted and phase of reflection arbitrary. The amplitude of the reflected wave is less than incident, and therefore when summed with the out of phase incident wave (as shown here), it is not nulled and will 'lift' the node (as shown in the upper panel) off the zero point.

is probably the easiest to understand. Figure 1 A & C are plots of the water depth (as measured by the height of 'wetness' on a stick placed at some distance r from the source). The matched load resembles the traveling wave, and the height of the wetness on the stick is the same for all r (Figure 1A). The perfectly unmatched and reflecting load features nodes that occur at $n\lambda/2$.

Most practical boundaries (or microwave devices) are neither perfect absorbers or reflectors and will therefore reflect a fraction of the incident wave. In such a case, you will find that the depth of the trough decreases in a manner that is commensurate with the amplitude of the reflected wave (Figure 1B). This is not intuitive from the wet stick model, so I'm going to have to drop that in favor of actual waveforms.

I have drawn perfectly reflecting waves in the top panels of Figure 2. The nodes appear at the half wavelength mark, and they are a minimum because even when the reflected wave is not begun at the crossing point the amplitudes of both incident and reflected wave are equal and cancel on average. If the reflected wave is less in amplitude than the incident, then the out-of-phase contributions don't cancel out on average, and one gets a net 'lifting' of the trough minimum.

The ratio of the standing wave maximum and minimum therefore can be used to specify the amount of reflected wave power or mismatch. One defines VSWR as D_{max}/D_{min} , and $1 < VSWR < \infty$. At no point thus far have I mentioned impedance. At high frequency the concept of impedance is arbitrary because the definition of voltage breaks down (voltage is defined as a line integral, which at high frequency becomes path dependent). This is the reason that matching and impedance at high frequency is defined in terms of wave reflection. The 50 ohm business that we so often encounter is arbitrary; it is a standard because, as it turns out, 50 ohm

transmission lines handle high power best and lose less of that power per foot (it's actually a compromise of two optimal values).

When designing a microwave or radiofrequency circuit, one therefore does not really have to get fanatical about impedance (I will qualify this statement below). A mismatch only affects the efficiency of your circuit, so one can, in principle, just haul out the really big amplifier to get you over the hump. This is why you can operate an ENDOR system without matching transformers or matching circuits and still get spectra. It's also why you can buy commercial microwave components off the shelf and tinker-toy them together to make a spectrometer. At the end, you only need a powerful enough source.

What keeps you from arbitrarily putting circuit elements together and compensating for losses by getting a truly huge amplifier is not impedance. Circuit design at high frequency is based on distributed network theory, in other words, size and geometry affect the behavior of the circuit element. The most straightforward examples are microstrip transmission lines that might accidentally have dimensions of a (fractional) wavelength and therefore resonate. The other example is the ENDOR coil that might experience some stray capacitance with the cavity wall, which likewise might resonate at some frequency.

Finally, insertion loss is defined as the log of the ratio of two powers delivered to a load, P_1 and P_2 . P_1 is the power delivered to a load when the device under test is not in the circuit; P_2 is the power delivered to the load when the device under test is in the circuit:

$$\text{Insertion loss} = 10 \log P_1/P_2 \text{ (dB)}$$

The important point to remember here is that the measured insertion loss depends on the impedance characteristics of the source and the load in the test circuit or system (these terms enter into the expression for power). The insertion loss that you measure or find in your spectrometer circuit may therefore not match the specifications; the agreement will depend on how similar the impedance properties of your system and the test circuit of the manufacturer.

NOTE: This Newsletter note and several others have recently been compiled and expanded for a chapter in a

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forthcoming *Biological Magnetic Resonance* volume. The chapter is entitled "Engineering Fundamentals for EPR Instrumentation" and is available as a preprint.

TIPS & TECHNIQUES

COMPUTER COUPLED ESR SPECTROSCOPY PROGRAM

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ABSTRACT

In recent years, Electron Spin Resonance (ESR) has been considered as an appropriate method for detecting irradiated food products to maintain regulatory control and to safeguard against fraudulent practices. The high cost of modern ESR instruments, however, limits the number of institutions world-wide who want to set up an appropriate laboratory to conduct the analysis. Fortunately, many institutions (especially university establishments) already possess older ESR instruments. This article is an extension to previous work undertaken in demonstrating the ease and inexpensiveness in the computerisation processes of older ESR facilities.

INTRODUCTION

The preservation and sterilisation of food by high energy ionising radiation have received much attention in recent years, especially in developing countries. As such, it is necessary to have adequate methods of detecting such food products to safeguard against fraudulent practices (Swallow, 1990). Electron Spin Resonance (ESR) is one such method and has gained much appraisal world-wide.

Modern ESR instruments, however, cost in the excess of £100,000 thereby limiting the number of institutions who want to set up an appropriate laboratory to conduct the analysis. The high cost is especially problematic for developing countries for three main reasons. Firstly, they

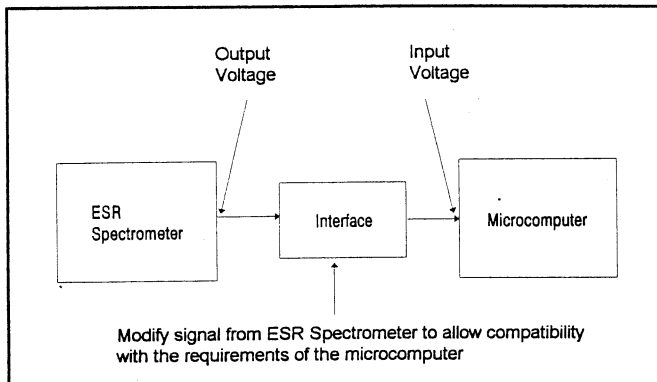


Fig. 1. ESR spectrometer - microcomputer interface.

need to buy irradiated food products because these products are cheaper than the normal unirradiated food products. Secondly, these products do not require complex storage processes that are lacking in these countries. Thirdly, high cost is a barrier to detecting the fraudulent practices that are common in these developing countries.

This article is an extension to previous work undertaken (Lee *et al.*, 1995) in demonstrating the ease and inexpensiveness in the computerisation processes of older ESR facilities. Lee *et al.* (1995) illustrate the construction of an interface to couple a BBC microcomputer (Model B) to an ESR spectrometer (Jeol JES-FE3X) to aid with the analysis. This article will present the flowcharts that highlights the essential features in writing the ESR spectroscopy program and the program listing itself. It must be noted that the interface and the program are designed for a Jeol JES-FE3X ESR spectrometer and a BBC Model B microcomputer, but where possible this article will highlight the general underlying principles in constructing the interface for other brands of ESR spectrometer and the increasingly popular IBM PC compatibles.

EXPERIMENTAL

ESR Spectrometer - Microcomputer Interface

To enable the spectra from the ESR spectrometer to be processed on the microcomputer, an interface between the two instruments is necessary.

As shown in Fig. 1, an interface is necessary to modify the signal from the ESR spectrometer to allow compatibility with the requirements of the microcomputer. Firstly, the output voltage of the ESR spectrometer must be identified. In the case of the Jeol JES-FE3X ESR spectrometer, this bipolar output voltage (from output terminal CN916) is ± 350 mV d.c. Second, the allowable input voltage to the internal analogue to digital converter (ADC) on the microcomputer must be identified. In the case of the BBC Model B microcomputer, the ADC accepts voltage signals ranging from 0 V to 1.8 V d.c.

To assist the reader, the interface circuit given in Lee *et al.* (1995) is presented in Fig. 2.

The interface circuit is designed for full-scale deflection (FSD) from the ESR spectrometer to be ± 350 mV d.c. and input voltage of the ADC on the microcomputer ranging from 0 V to 1.8 V d.c. Most older brands of ESR spectrometer have FSD of approximately ± 500 mV d.c. The most commonly used microcomputers - IBM PC compatibles - accept input voltage ranging from 0 V to 12 V d.c. from the RS232 serial port. For accuracy, it is important to utilise the maximum ESR output voltage and the maximum microcomputer input voltage.

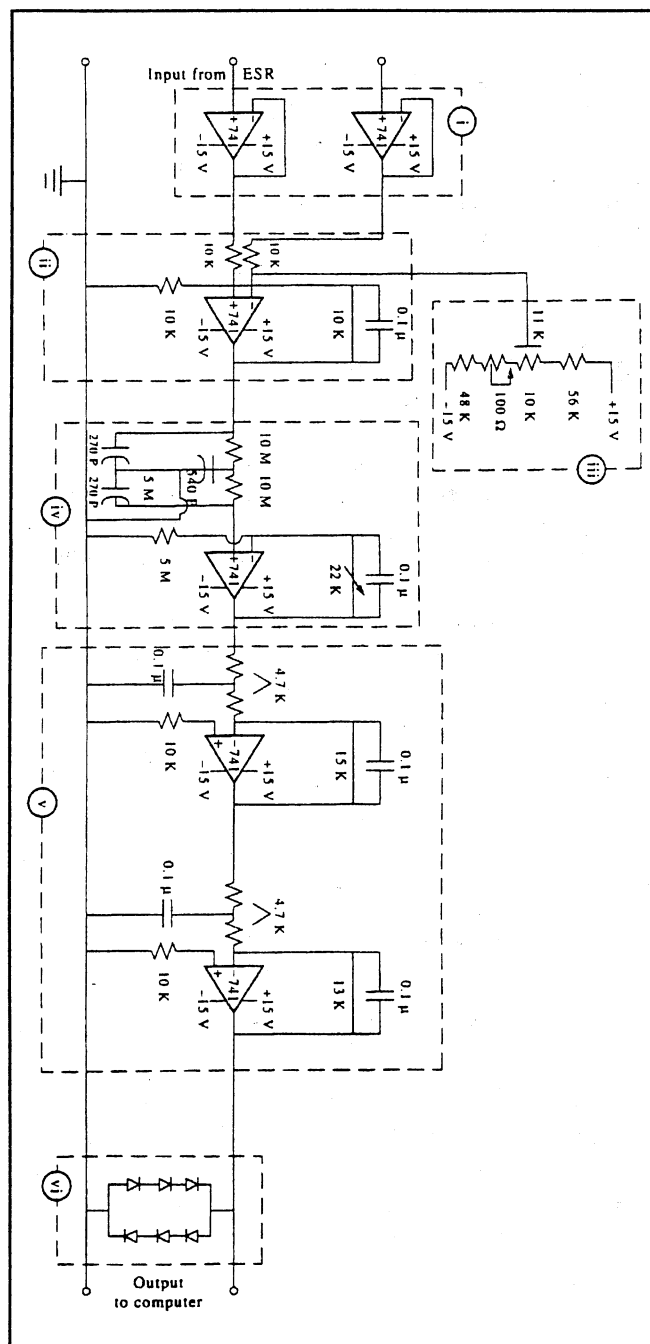


Fig. 2. Circuit diagram for ESR spectrometer - BBC microcomputer interface.

IBM PC compatibles (minimum specification: 386 DX33 processor, 4 Meg RAM, 120 Meg Hard Disk, 1 Meg SVGA Graphics Card, SVGA Colour Monitor) have many advantages over older computing facilities such as the BBC Model B microcomputer. The following are some of the most important features:

- faster processing time,
- larger input ADC voltage for accuracy,
- higher screen resolution for more accurate positioning and calculation of B- and g- values,
- larger storage capacity of spectra, and
- most widely used microcomputer in Europe and Asia - fruitful for data sharing on the increasingly popular Internet.

To use the IBM PC compatibles, several modifications are necessary to the original interface circuit designed for a Jeol JES-FE3X ESR spectrometer and a BBC Model B microcomputer. The amplification part of the circuit (part ii) needs to be altered to take the voltage to approximately 10 V instead of 1.8 V. To protect the ADC on the IBM PC compatible, the diode limiter part of the circuit (part vi) also needs to be changed to give 12 V instead of 2.4 V. Any offset voltage can be fine tuned by altering the potentiometer in part iii of the circuit. For a more detailed description on the construction of the interface see Lee (1990).

ESR Spectroscopy Program Flowchart

Although the ESR program listed in Appendix 1 was written in BASIC for use with the BBC Model B microcomputer, the general programming methodology, as shown by the flowchart in Fig. 3, can be used for other programming languages such as Turbo Pascal, Turbo C++, Fortran 77 or Visual BASIC.

As shown in Fig. 3, the ESR program is organised into 7 parts. The main menu acts as 'control panel' to access other parts of the program. Each part is independent from one another, but validity checks have been implemented. For example, the program will not allow the user to output a spectrum prior to loading that spectrum from a disk file or to recording it.

After recording the first spectra, the user has a choice to save the spectra for future usage, to output the spectra onto the screen or printer, to analyse the spectra, or to exit the program. The analysis option is further divided into 6 parts where the user can choose between zooming into a region of interest of a particular spectrum, reducing the spectra for a full view, superimposing two or more spectra, subtracting spectra, calculating B- and g- values that correspond to the positioning of the cursor keys, or returning to the main menu.

The program is designed such that further options can be added to the program without interfering with the structure of the program. Additional options can be written separately and access to them is controlled via the main menu.

Note that if IBM PC compatibles are to be used, then the number of data points can be increased for further accuracy. The number of data points is a limiting factor on the BBC Model B microcomputer because of the relatively small on-board memory. It must be noted that if the number of data points is set too large, then the spectra would appear to have more 'noise' and thus defeat the original objective to increase the accuracy. It is sensible to keep the number of data points to less than 1200.

ESR Spectroscopy Program Listing and Documentation

The full ESR program listing is given in Appendix 1. Please note that documentation on the right hand side of the listing is presented to assist the reader. The remarks are in addition to the 'REM' statements given in the program and have nothing to do with the program itself. Please also note that the use of 'GOTO' and 'GOSUB' statements in BASIC have been minimised. Programmers with a preference for other programming languages to BASIC can simply translate the program listing to the corresponding syntax of that language.

CONCLUSIONS

This article is an extension to previous work undertaken (Lee *et al.*, 1995) in demonstrating that the application of coupling a BBC microcomputer to the ESR spectrometer has been a valuable tool in facilitating the processing of spectra, and in the acquisition and storage of data. The general features to couple the more powerful and commonly used

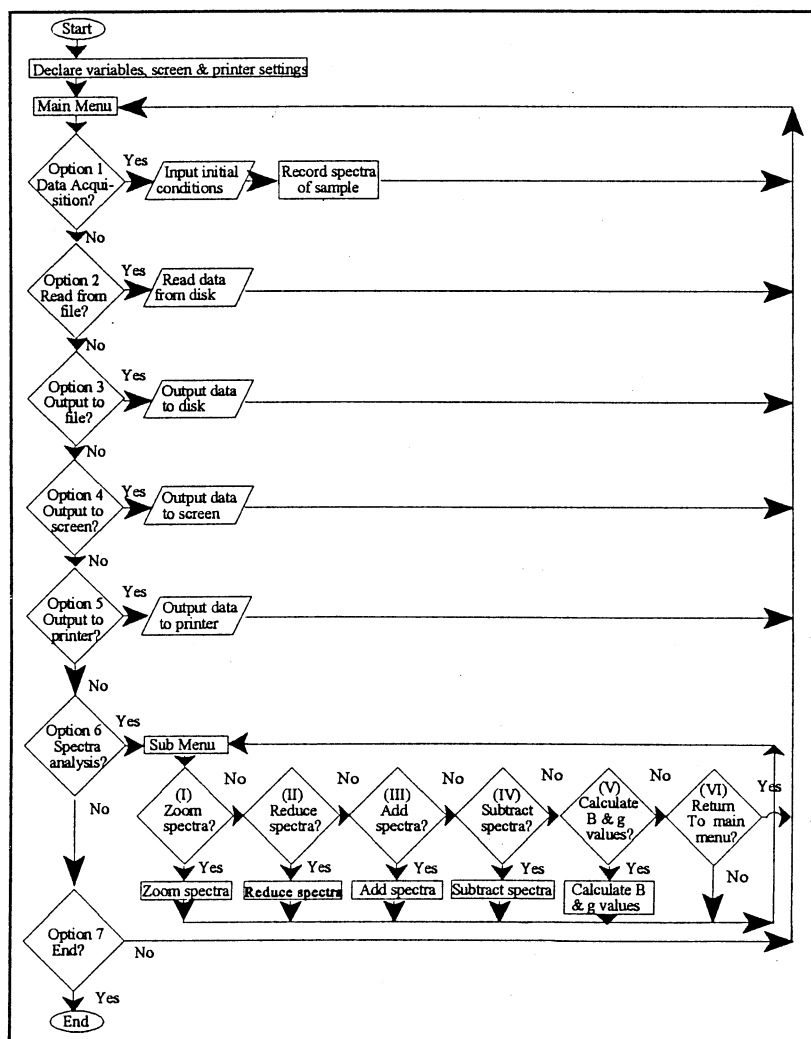


Fig. 3. ESR program flowchart.

IBM PC compatibles to other brands of ESR spectrometer have also been given.

The approach employed is inexpensive, easy to implement, and makes use of existing technology. The end result is argued to be comparable (if not fully equal) to modern ESR instruments in terms of the quality of spectra obtained. The cost for the implementation is negligible compared with purchasing a new ESR spectrometer or upgrading recent models.

I hope that institutions, especially in developing countries, that possess older ESR instruments can benefit from the approach given here, at least until they can afford to acquire the elegant computer-wise EPR spectrometers that the EPR Newsletter advertisers offer. I also hope that institutions can place their valuable ESR spectra data on the increasingly popular Internet for others to share and to benefit from one another. To finish on a proverb: 'a wise man learns from experience and an even wiser man from the experience of others' (Plato, 1974).

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APPENDIX 1: ESR Spectroscopy Program Listing and Documentation - The program and documentation are available on the IERC (Illinois) ftp server or from the EPR

Newsletter World Wide Web homepage -
<http://ierc.scs.uiuc.edu/news.html/>.

BOOKS & JOURNALS

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"Applied Magnetic Resonance" publishes original articles with a strong emphasis on new applications of the technique and on new experimental methods. Routine applications to structural chemistry are outside the scope of the journal. Review articles are invited on methods and applications of NMR, NQR, EPR, Mössbauer spectroscopy, etc. A section is devoted to book reviews and Letters to the Editor. Information on conferences and new technical equipment are also accepted.

The Editorial Board and Advisory Board of AMR provide a perfect balance between various fields of magnetic resonance as well as between different countries and universities and research centers. The support and efforts of the members of the Editorial and Advisory Boards are very important for the success of "Applied Magnetic Resonance".

Five years ago, I formulated two main considerations in favour of AMR. The impressive variety of applications of magnetic resonance methods and their penetration into new fields of science and technology called for the appearance of a journal targeted at this, so as to stimulate the expansion of applications of magnetic resonance. No less important was the expectation that this journal would bridge the gap between scientists from East and West. As envisioned, the joint and the juxtaposed work within one journal would expand the international collaboration of scientists and would strengthen interdisciplinary bonds.

At present, such collaborations of scientists from the former Soviet Union with their Western colleagues are indeed successfully developing, and I firmly believe that our journal contributes to this collaboration.

I am pleased that this journal finds its way to the international magnetic resonance community. We have had successful presentations of the journal during various conferences, the ENC in St. Louis 1993 and in Boston 1995,

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the 26th Congress AMPÈRE 1992 in Athens and the 27th Congress AMPÈRE 1994 in Kazan to name a few. A flow of high-quality regular papers continuously increases.

We have had a number of very interesting special issues dedicated to specific fields of magnetic resonance and mainly demonstrating the momentary slice of the state-of-the-art. And I am most grateful to the guest editors for their efforts in preparing these special issues and involving new enthusiastic people in the AMR activity. I am happy to name all of them (chronologically): C. von Borczyskowski "Optical Detection of Magnetic Resonance in Solids", J.A. Weil and M.K. Bowman "EPR in the Determination of Structure", M. Mehring "Magnetic Resonance in High-Tc Superconductors", M. Brustolon and C. Corvaja "Recent Advances in ESR Spectroscopies. Applications to Chemistry, Physics and Biology", M.E. Smith "²⁷Al Solid State NMR", V.D. Fedotov "Magnetic Resonance and Dynamics of Proteins", H.M. Vieth and C. von Borczyskowski "Non-Thermal Nuclear Polarization", N.D. Yordanov "Quantitative EPR Spectroscopy", Yu.D. Tsvetkov "ESR Pulsed Radiospectroscopy and its Applications", R.I. Zhdanov and R. Kaptein "Study of Nucleic Acids and their Interactions Using Magnetic Resonance Methods", J. Stankowski "Magnetic Resonance and Microwave Absorption in High-Tc Superconductors and Fullerenes", and J.B. Miller "NMR in Noble Gases".

In 1994 a special issue of AMR was dedicated to the 50th anniversary of the discovery of electron paramagnetic resonance by E.K. Zavoisky. Lectures of the Zavoisky Awardees are also published in AMR.

Forthcoming special issues on selected topics under the guidance of guest editors are as follows: N.D. Yordanov "Quantitative EPR Spectroscopy", E. Roduner "Muon Spin Spectroscopy", K.-P. Dinse "EPR in Fullerenes", L. Kevan "Magnetic Resonance in Porous Media", K. Möbius and D. Stehlik "EPR in Studying Photosynthesis". However, I would like to encourage the contributors to send their regular papers to our journal. These special issues do not hinder in any way prompt publication of regular papers. Usually the papers are published in six months.

AMR is now indexed/abstracted in: Current Contents, Current Awareness in Biological Sciences, Sci Search, Research Alert, Chemistry Citation Index, INSPEC. In the end of 1995 its IMPACT factor will be announced.

It is my pleasure to emphasize that the publishers, Springer-Verlag Wien New York, demonstrate complete understanding and true collaboration during all these years. *I particularly mention that Springer has a special subscription rate for members of the EPR(ESR) Society, members of the AMPÈRE Society, and members of ISMAR (US \$ 92.00 plus US \$ 40.00 postage).* I hope that this proposal will increase the number of individual subscribers to AMR. Let "Applied Magnetic Resonance" become your guide in the expanding world of applications of magnetic resonance.

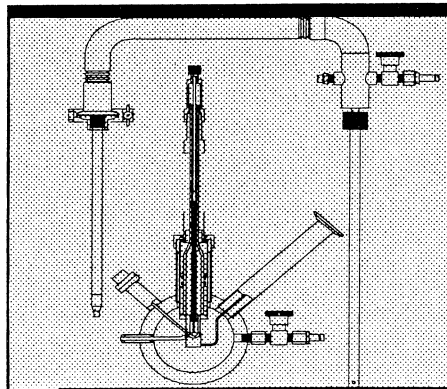
I am very grateful to all colleagues who submit manuscripts, referee them, subscribe to AMR etc.

Kev M. Salikhov, AMR Editor
Zavoisky Institute, Kazan

"EMR of Solid State" Volume Now Available at a Reduced Rate to IES Members

The Canadian Society for Chemistry has made a number of copies of its volume *Electronic Magnetic Resonance of the Solid State* available to members of the International EPR Society at US\$60. At a discount of 1/3 off the regular international price of US\$90, this volume will be a handsome and informative addition to your reference collection. Produced in 1987, *Electronic Magnetic Resonance of the Solid State* contains 43 review articles written and refereed by leading authorities in the field. The volume covers most aspects of EPR spectroscopy, ranging from theory through structural studies, multiple resonance techniques and time-resolved spectroscopy to the very latest in EPR imaging.

To obtain your copy, please contact the Publications Department, Canadian Society for Chemistry, 130 Slater St., Suite 550, Ottawa, ON, CANADA K1P 6E2. ☎: 1-613-232-6252; FAX: 1-613-232-5862.



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CONFERENCE REPORTS

IVth INTERNATIONAL WORKSHOP "ELECTRON MAGNETIC RESONANCE OF DISORDERED SYSTEMS" and 1st INTERNATIONAL SEMINAR "APPLIED EPR", held June 12-19, 1995, in Sofia-Bojana, Bulgaria, were organized by the BULGARIAN EPR SOCIETY in collaboration with the Institute of Catalysis, Bulgarian Academy of Sciences, and the Department of Chemistry, Sofia University. The meetings were sponsored by BRUKER Analytische Messtechnik, GmbH and National foundation "Scientific Research". The aim of the EMARDIS workshop is to cover all qualitative (structure-reactivity, kinetics, etc.) aspects of recent development in theory, experiment, methodology, instrumentation, etc. of EMR (EPR, ENDOR and ESE) spectroscopy of disordered systems through (1) lectures given by top specialists and selected applicants and (2) round-table discussions. The APPLIED EPR seminar was planned to cover: Fundamental aspects of Quantitative EPR (standards, calibration, metrology and methodology of quantitative measurements, instrumentation - new methods, advanced techniques, automation, etc.); EPR Dosimetry (monitoring of high energy radiation effects, high energy radiation processing control in food preservation and sterilization, dating of archeological and geological samples, etc.); EPR in medicine (clinical and biomedical studies); EPR in the environmental control; EPR in petrol industry; EPR in geology (mineralogy, petrology and fossil fuels); EPR in polymer chemistry, etc.

To facilitate interaction, each of these meetings was limited to about 35 to 40 persons and was conducted somewhat like a Gordon Conference. All participants lived, dined, lectured, and conversed in a hotel situated in Mounth Vitosha, about 10 km away from Sofia downtown. The general scheme of both meetings was: Opening: Monday - welcome party after arrival and transportation to conference site. Working EMARDIS workshop days: Tuesday - Thursday morning. Tourist and social events: Thursday - sightseeing in Sofia, farewell dinner in the evening. Friday - excursions (to Rila or Batchkovo Monastery) for those staying to attend the 1st International seminar on "Applied EPR" or departure/arrival day for participants who attended only one of the meetings, followed by Welcome party for the "Applied EPR" attendees. Working APPL-EPR days: Saturday/Sunday, with Sofia sightseeing Saturday afternoon.

Special event: During the APPL-EPR meeting (June 17), all celebrated the 63d birthday of Masamoto Iwaizumi at a

reception given by the Bulgarian EPR Society. APPL-EPR Conclusion: Breakfast Monday following a farewell dinner on Sunday evening.

Representatives from 20 countries of America, Asia and Europe (Australia, Austria, Belgium, Canada, China, France, Germany, Hungary, India, Israel, Japan, Mexico, Poland, Portugal, Russia, Switzerland, The Netherlands, UK, USA and Bulgaria) attended.

EMARDIS lectures: The following distinguished specialists delivered lectures during EMARDIS sessions: J. Forrer - *Recent developments and investigations of pulsed ESE/ENDOR spectrometers*; C. Friebel - *A classical EPR study of cooperative orderings of the pentaammine-copper(II) polyhedra in $Cu(NH_3)_5X_2$ compounds ($X = Br, BF_4, ClO_4$)*; E. Giamello - *The interaction between hydrogen peroxide and metal oxides: EPR investigations*; D. Goldfarb - *The nature of the distal axial ligand in Cytochrome P450 as studied by ^{17}O and 1H ESEEM and pulsed ENDOR spectroscopies*; G. Grampp - *Measurements of electron transfer rates by EPR line-broadening effects*; A. Hoff - *Multifrequency EPR and ENDOR on specifically ^{13}C -labeled tyrosines in vitro and in the reaction center of photosystem II of plants*; G. Jeschke - *Hyperfine correlated chirp ENDOR spectroscopy*; H. Kaess - *EPR, ENDOR and ESEEM Studies of photosynthetic reaction centers*; H. Kurreck - *Mimicking primary processes of photosynthesis-model compounds, light-induced charge separation*; Ya. S. Lebedev - *EPR of triplet- and quartet-state species in disordered systems: Thermal spin polarization and spin diffusion effects*; V. Beltran-Lopez - *Complete theoretical EMR powder spectra by the isotimic method*; G. Maresch - *Application of CW and pulsed 94 GHz EPR spectroscopy to synthetic polymers*; S. K. Misra - *Interpretation of Mn^{2+} EPR spectra in disordered materials*; Y. Ohba - *Spin relaxation studies of metallofullerene $La@C_{82}$ by FT- and CW-EPR spectroscopy*; J. Pilbrow - *Some new strategies in CW and pulsed EPR*; B. S. Prabhanda - *Inferring unresolved EPR hyperfine structure in solutions*; E. J. Reijerse - *Multifrequency and multidimensional ESEEM strategies for studying metal-nitrogen interactions*; A. Rockenbauer - *Automatic computer simulation of ESR spectra*; J. Stankowski - *ESR and MMR study of C_{60} upon K-doping process. Two Tc of superconducting phase transition*; S. van Doorslaer - *^{31}P and 1H powder ENDOR study of ozonide radicals in carbonated apatites, synthesized from aqueous solutions*; H. van Willigen - *FT-EPR study of photoinduced electron transfer reactions in microheterogeneous media*; Y. Xu - *Studies on EPR & ENDOR spectra of ^{14}N and ^{15}N labeled bis(2-hydroxyacetophenyl-ketoxime) $^{63}Cu(II)$ & $^{65}Cu(II)$ complexes in disordered systems*; O'Neil P. Braganza, B. S. Prabhanda -

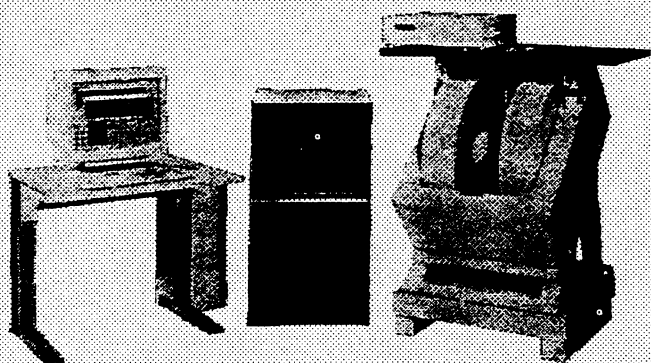
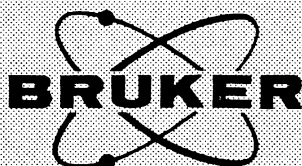
Circuit module for selective magnetic field scanning in magnetic resonance spectrometers.

A Round Table Discussion on: "Trends in computer simulations of EMR spectra of disordered systems" was organized Wednesday evening.

APPL-EPR lectures: The following specialists delivered expert lectures on the days devoted to APPL-EPR: R. Czocho - *Quantitative EPR - sensitivity to experimental conditions and optimal setting of recording parameters*; K. Dyrek - *Quantitative EPR studies of transition metal ions in oxide, aluminosilicate, and polymer matrices*; M. Iwaizumi - *Two-dimensional FT-EPR nutation spectroscopy of spin-correlated radical pairs*; J. Pilbrow - *CW & Pulsed EPR in Materials Science*; J. Raffi - *EPR detection of irradiated foodstuffs*; G. Rist - *ESR and CIDNP investigation of industrial additives*; E. Stewart - *Detection of irradiated crustacea using EPR spectroscopy including the results of an interlaboratory trial*; A. M. Wasserman - *Some EPR spin probe and spin label studies of polymer systems*; Y. Xu - *Electronic structure of low-dimension bridged polar coordination complex polymers and their possible prospect as the material of NLO studied by EPR*; T. Budinova - *EPR investigation of oxidized anthracite*; R.

Kostov - *Mineralogical-genetic atlas of electron-hole centers in natural quartz*; N. D. Yordanov - *Is our knowledge about DPPH enough to appoint it as a primary standard for quantitative EPR spectrometry?*

Poster sessions: EMARDIS – J. Forrer, S. Pfenninger, G. Jeschke, M. Hubrich, B. Wagner, T. Weiland, A. Schweiger - *Time-resolved field distribution, efficiency, and performance of pulsed ESE/ENDOR probeheads*; G. Gencheva, N. Mincheva, M. Miteva - *Paramagnetic palladium complex with amide-containing ligand biuret*; G. Gochev, N. D. Yordanov, T. Kurisaki, H. Wakita - *Simulation of the EPR spectra of copper(II) complexes with anisotropic shf interaction*; B. G. Jeliazkova, M. A. Doicheva, L. B. Tosheva - *EPR study on the chemistry and photochemistry of copper(II) dithiocarbamate mixed-ligand complexes*; B. G. Jeliazkova, M. A. Doicheva, L. B. Tosheva - *Thermodynamics of ligand exchange reactions between bis(dithiocarbamate)Cu(II) and CuX₂. An EPR study*; B. G. Jeliazkova, G. Ch. Sarova - *EPR study on the photoinduced electron transfer in the ternary complex (dithiocarbamate, dithiophosphato)copper(II)*; N. Nedelchev, N. D. Yordanov - *IBM PC controller for Bruker ER250 ENDOR system*; P. J. van Dam - *A multifrequency*



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ESEEM study of Cu(II)Bleomycin and related model compounds; N. D. Yordanov, N. Patev - EPR study on bis(b-diketonato)copper(II)- solute-solvent interactions; N. D. Yordanov, E. Vasileva, E. Ganeva - EPR study of bis(dithiocarbamato)Ag(II) complex in the presence of some quaternary alkylammonium salts; N. D. Yordanov, M. Zdravkova - EPR studies of gamma-irradiated dithiophosphates. APPL-EPR - R. Kostov, Y. Yanev - EPR data of volcanic siliceous glasses from the Eastern Rhodopes (Bulgaria) and the Lipari island (Italy); N.D. Yordanov, R. Christov, B. Veleva - EPR study of aerosols with carbonaceous products in urban air; N.D. Yordanov, P. Slavov - Effect of diameter and wall thickness of quartz pipe inserted in EPR cavity on signal intensity.

Proceedings: All main lectures from both meetings as well as a selection from the original short communications will be published in a special issue of Applied Magnetic Resonance (planned for vol. 10, issue 1-2, 1996).

The next EMARDIS meeting with its specific extension is planned for 1997. Contact person: Nicola D. Yordanov, Institute of Catalysis, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria, tel.: (+3592) 713 2546, 713 3917 or 724917, fax: (+3592) 756116 or 720038, E-mail: ndyepr@bgearn.bitnet or ndyepr@bgearn.acad.bg.

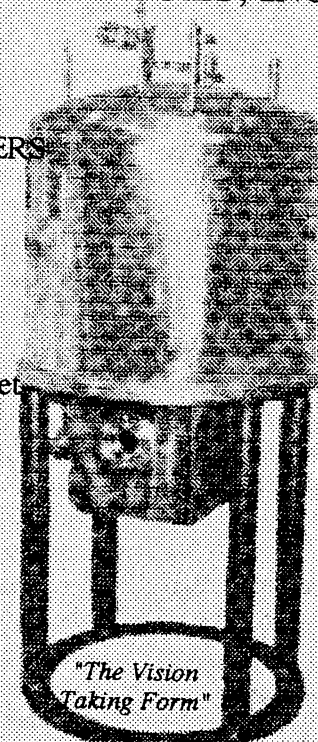
ZAVOISKY AWARD EVENTS, 1995

The Annual 1995 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was presented to Professor James S. Hyde in a ceremony marking his outstanding contributions to the development of instrumentation and methodology of electron paramagnetic resonance spectroscopy. This ceremony was preceded by the Fourth Annual "Modern Development of EPR" Workshop, 28-29 September, 1995. The program of the Workshop was as follows: J.S. Hyde (Milwaukee) "Multiquantum EPR, ENDOR and ELDOR"; Ya.S. Lebedev (Moscow) "EPR of High-Spin Complexes Formed under Mechano-Chemical Treatment"; V.A. Goncharov, I.V. Ovchinnikov (Kazan) "Time-Domain Reflectometry in Magnetic Resonance: Lumped-Inductance Method"; C. von Borczyskowski (Chemnitz) "Hyperfine Interaction of a Single Electron Spin"; I.A. Gromov, S.B. Orlinskii, R.M. Rakhmatullin (Kazan) "ESEEM of Rare-Earth Ions at X- and Q-bands"; L. Kevan (Houston) "Pulsed ESR Studies of Transition Metal Ions in Microporous Materials"; M.S. Tagirov, H.P. Moll, D.A. Tayurskii, J. van Tol, P. Wyder (Kazan, Grenoble) "High Magnetic Field Investigation of Tm³⁺ Ions in Ethylsulfate Crystals"; B.Z. Malkin, R. Yu. Abdulsabirov, S.L. Korableva, G.S. Shakurov, A.L. Stolov,

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V.F. Tarasov, A.V. Vinokurov (Kazan) "Submillimetre EPR Spectroscopy of Van-Vleck Paramagnets in Parallel Fields".

The Zavoisky Award was presented September 29, 1995 in the capital city of the Republic of Tatarstan Kazan. It was there that Academician E.K. Zavoisky discovered EPR in 1944. The Zavoisky Award consists of a Diploma, a Medal and one thousand US dollars.

The Zavoisky Award was established by the Zavoisky Physical-Technical Institute of the Russian Academy of Sciences with support from the Kazan State University, the Springer-Verlag Publishing House, the Republic of Tatarstan, the Tatarstan Academy of Sciences, the AMPÈRE Society and the International EPR Society. The Award Selection Committee consisted of well-known experts in EPR: Professors 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).

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

The selection of Professor James S. Hyde was made from many nominations solicited from international experts in EPR.

In the morning of September 27, a reception for Professor James S. Hyde and his wife by the Prime Minister of the Republic of Tatarstan F.Kh. Mukhametshin took place.

The Award Ceremony starting in the afternoon of September 29 was attended by over 200 people, among them were the scientists who had participated in the preceding Workshop. Delegation of the Department of General Physics and Astronomy of the Russian Academy of Sciences participated in the Award Ceremony. Professor Yu.A. Sherstkov (Ekaterinburg), Academician Professor K.A. Valiev (Moscow), Professor R.K. Mazitov (Moscow), and Professor A.A. Manenkov (Moscow) were also present.

The ceremony was chaired by Deputy Prime-Minister of the Republic of Tatarstan I.K. Khairullin. The Chairman of the Award Committee, Professor K.M. Salikhov announced the decision of the Zavoisky Award Committee. The presentation was made by Professor V.N. Likhachev, the Chairman of the State Council of the Republic of Tatarstan. The President of the Tatarstan Academy of Sciences Professor M.Kh. Khasanov, the President of the Kazan Scientific Centre of the Russian Academy of Sciences Professor I.A. Tarchevskii, Dr. V.A. Zayats, on behalf of the President of the Russian Academy of Sciences, and the Deputy Rector of the Kazan State University Professor B.N. Solomonov warmly congratulated the laureate. The letters of congratulations from Professor R. Kind, Secretary General of the AMPÈRE Society, Professor A. Schweiger, Secretary of the International EPR Society, and Professor G. Laukien, Chairman of the Board Bruker-Physik were handed to Professor James S. Hyde.

J.S. Hyde gave his Zavoisky Award lecture in which he shared memories about his previous trips to Kazan, Moscow and Novosibirsk, discussed the evolution of design of bimodal resonators, and closed with a few personal slides. A concert by a 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 the Kazan State University. A choral concert followed to mark the event which was concluded with a Banquet in honor of



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Prof. James S. Hyde and his outstanding contributions to EPR. During a stay in Kazan the laureate and his wife visited the Raifa monastery, and the ancient fortress and the monastery in the Sviyajsk island on the Volga river.

NOTICES OF MEETINGS

**ASTM SUBCOMMITTEE E10.01, HYATT
REGENCY PEACHTREE CENTER, Atlanta, GA,
Jan 30-Feb 1, 1996.**

The ASTM is the American Society for Testing and Materials, organized in 1898, as a not-for-profit voluntary standards development system. ASTM Headquarters has no technical research or testing facilities; such work is done voluntarily by 34,500 technically qualified ASTM members located throughout the world. Membership in the Society is open to all concerned with the fields in which ASTM is active. Additional information may be obtained from the ASTM, 1916 Race St., Philadelphia, PA 19103; ☎: 1-215-299-5454.

The ASTM Committee E10 on Nuclear Technology and Applications is divided into several subcommittees, of which Subcommittee E10.01 is concerned with Dosimetry for Radiation Procession and is the Subcommittee of interest to EPR Spectroscopists involved in dosimetry and radiation effects on matter. The Subcommittee meets in January and June and has completed 18 internationally recognized standards for radiation dosimetry published in the ASTM's

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Annual Book of Standards, Section 12, Volume 12.02 Nuclear(II), Solar, and Geothermal Energy.

Standards currently being revised or formulated include "Standard Practice for Use of the Alanine-EPR Dosimetry System" E-1607-94 and "Standard Practice for Blood Irradiation Dosimetry" E 10.01X.

The next meeting will be held at the Hyatt Regency Peachtree Center in Atlanta, GA between Jan. 30 and Feb. 1, 1996. The Chairman of the Subcommittee and the person to contact for more information is Dr. Harry Farrar IV, 18 Flintlock Lane, Bell Canyon, CA 91307-1127, ☎: 1-818-340-1227, FAX: 1-818-340-2132.

ESR SPECTROSCOPY OF INORGANIC RADICALS AND METAL IONS IN INORGANIC AND BIOLOGICAL SYSTEMS, Edinburgh, Scotland, March 24-28, 1996.

The 29th meeting of the ESR Group of the Royal Society of Chemistry, London will celebrate 28 consecutive years of International Meetings on the topic of Electron Spin Resonance Spectroscopy. The meeting will be held at The University of Edinburgh. The conference opens with a reception and dinner on Sunday evening and closes after lunch on Thursday. The organizers take pleasure in extending a cordial invitation to all persons interested in ESR spectroscopy in Chemistry, Physics and Biology to attend. Accommodation will be in individual rooms in a Hall of Residence on the campus, where the lectures will take place.

Scientific Program: The following have accepted invitations to present lectures: R.C. Bray (Univ. Sussex), *EPR and Related Studies of Transition Metals in Enzymology: Are They Worth the Trouble?*; D. Gatteschi (Univ. Florence), *High Frequency EPR Spectra of Larger Magnetic Clusters*; B.M. Hoffman (Northwestern Univ.), *The Bruker Lecture: ENDOR of Metalloenzymes*; J.W. Ingledew (Univ. St. Andrews), *Bimetallic Sites in Biological Processes*; W. Lubitz (Technical Univ. Berlin), *EPR and ENDOR Studies of the Water-Oxidizing Complex in Photosynthesis and of Related Model Systems*; J. Morton (Steacie Inst., Ottawa), *The Addition of Organic and Inorganic Radicals to C60: an ESR Study*; R. Riedie (Univ. St. Andrews), *Developments in ESR Spectrometers and Spectroscopy at Frequencies above 90 GHz*; D.J. Singel

(Montana State Univ.), *ESEEM and High-Field EPR Studies of the Oncogene Protein ras p21*; A.I. Smirnov (Univ. Illinois C-U), *95 GHz ESR of Biological Systems*; D.H. Whiffen (retired), *Personal Memories of ESR and ENDOR 1956-1968*.

Social Program: The following social activities have been planned: Sunday evening: Welcome Reception; Monday evening: Whisky Tasting; Tuesday afternoon: bus tour of Edinburgh; Tuesday evening: Wine reception after Bruker Lecture; Wednesday evening: Reception and Conference Dinner.

Abstracts: Those wishing to submit a poster must send details of their contribution, typed neatly on one sheet of A4 size paper (30 x 21 cm) giving title, authors, name of institution and abstract. Please state whether you wish to submit a full paper, based on your poster, to be considered for publication in a Journal of the Chemical Society. Abstracts should be sent no later than January 8, 1996 to Dr. C.C. Rowlands, Dept. Chemistry, Univ. Wales Cardiff, P.O. Box 912, Cardiff CF1 3TB, Wales, UK. Abstracts will be reproduced for distribution to all participants. The authors of posters will be advised as soon as possible after February 1, 1996 about the method of presentation.

Conference Proceedings: All contributors to both talks and posters are invited to submit the contents of their paper (if previously unpublished) for publication in a Journal of the Chemistry Society. The issue will be sent to all participants.

Bruker Lectureship: Bruker Analytische Messtechnik GmbH generously sponsors an annual Lecture to be given by a scientist who has made major contributions to the development and use of ESR spectroscopy. This year, the Lectureship has been awarded to Professor B.M. Hoffman.

The Committee of the ESR Group, Royal Society of Chemistry consists of: Prof. C.J. Rhodes (Chairman), Dr. C.C. Rowlands (Secretary), Prof. A.G. Davies FRS, Dr. S.A. Fairhurst, Dr. R.A. Jackson, Dr. D. Lowe, Dr. F.E. Mabbs, Dr. J.B. Raynor, Prof. L.H. Sutcliffe, Dr. J.C. Walton. The Local Organiser is Dr. L. Yellowlees. Dr. Rowlands' e-mail address is sacccr@cardiff.ac.uk.

The circular may also be viewed on the Internet at the following World Wide Web address:

<http://www.cf.ac.uk/uwcc/chemy/trowlandsc/conf.html>

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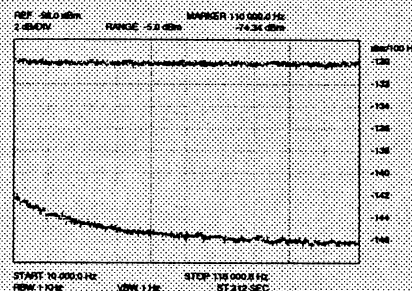
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**THE FOURTEENTH INTERNATIONAL
CONFERENCE ON RADICAL IONS, Uppsala,
Sweden, July 1-5, 1996.**

The Radical Ions conference is a continuation of previous Gordon Conferences 1968-1992 (totally 12) and the corresponding conference held in Halifax in 1994. Following our traditions, the conference will feature invited speakers and poster sessions with time for informal discussions. There will also be space for a number of short oral presentations.

The meeting will take place in the main building of Uppsala University, built in the center of Uppsala in the end of the last century. Uppsala is centrally located in Sweden, with excellent connections both by air (Arlanda airport), by train and by car.

The invited and contributed papers will be published in Acta Chemica Scandinavica as Minireviews, Articles or Short Communications, whichever is appropriate, and will be collected into a bound Symposium volume by the organizers. Regular refereeing procedures will be applied.

A significant part of the studies to be presented will involve EPR as a tool. Topics to be covered in the invited talks include:

- Spectroscopy and matrix isolation techniques.
- Radical ions in photochemistry and radiation chemistry
- Synthetic applications of radical ions
- Radical ions on surfaces
- Radical ions in biological systems
- Radical ions in electrochemistry
- Quantum chemical techniques

The registration fee is \$250 for active participants. The cost for a first class hotel, centrally located, is approximately \$70/night, breakfast buffet included, but there are cheaper accommodations in student dormitories that can be arranged. The total number of participants is limited to about 100. Acceptance will be on a first-come, first-served basis. More details are available in a first circular that will be distributed

to those interested in attending the conference. To obtain the circular, contact Mari Lofkvist, Secretary, RADICAL IONS 14, Department of Physics, IFM, Linköping University, S-581 83, Linköping, Sweden. For further information about the scientific programme please contact one of the chairmen: Anders Lund, Dept. Physics, IFM, Chemical Physics Laboratory, Linköping Univ., S-581 83, Linköping, Sweden, FAX: 46-13-13-22-85, E-mail: ald@irm.liu.se; Sten Lunell, Dept. Quantum Chemistry, Box 518, Uppsala Univ., S-751 20, Uppsala, Sweden. Or communicate by FAX or E-mail: FAX: 46-18-50-24-02, E-MAIL: lunell@kvac.uu.se.

**NINETEENTH INTERNATIONAL EPR
SYMPOSIUM at the 38th Annual Rocky Mountain
Conference, Denver, CO, USA, July 21-25, 1996.**

For more information contact: Prof. Sandra S. Eaton, Univ. Denver, Dept. Chemistry, Rm. 153 Seely G. Mudd Science Bldg., Denver, CO 80208, USA; ☎: 1-303-871-3102; FAX: 1-303-871-2254; E-mail: seaton@du.edu or Prof. Gareth R. Eaton, Univ. Denver, Dept. Chemistry, Denver, CO 80208, USA; ☎: 1-303-871-2980; FAX: 1-303-871-2254; E-mail: geaton@du.edu.

**XVIIth INTERNATIONAL CONFERENCE ON
MAGNETIC RESONANCE IN BIOLOGICAL
SYSTEMS, Keystone, Colorado, USA, August 18-23,
1996.**

This is the first meeting in this biennial series to be held in North America since 1988.

Conference Program. A broadly based program has been planned, covering new magnetic resonance methods, applications of high resolution NMR to structural biology, application of solid state NMR techniques, use of EPR in studying a variety of paramagnetic systems, *in vivo* spectroscopy and imaging, and a minisymposium on Biomolecular NMR and Drug Discovery. The conference will feature 12 plenary lectures, along with about 80 invited lectures and 25 short talks in three parallel sessions. Three poster sessions, each accommodating up to 200 posters, will permit participation by a large number of workers active in many aspects of biological magnetic resonance.

Conference locale. The meeting will be held at the Keystone Conference Center, which has been the site of several conferences on protein NMR. Keystone is a planned resort community in the Rocky Mountains, about 75 miles west of Denver. Most air travelers will fly to the new Denver International Airport, which has good domestic and international connections. Rental cars and shuttle buses are available from the Denver Airport to Keystone. The Conference Center, opened in 1989, will be the site of all lecture and poster sessions, with coffee breaks and display of vendor materials in the foyers and terraces. The nearby Keystone Lodge will provide space for commercial exhibitors and hospitality suites. The Keystone Resort includes two hotels, with 255 rooms, as well as 800 condominium units. There are many restaurants in all price ranges and full recreational facilities for swimming, boating, golf, tennis, hiking and trail riding. During August the

weather at Keystone is usually very pleasant, with daytime high temperatures running 20°-30°C.

For further information, contact the Conference Office, attn: Judith A. Sjoberg, Conference Manager, at 1201 Don Diego Ave., Santa Fe, NM 87505 USA; ☎: 1-505-989-4735; FAX: 1-505-989-1073. A page has been established on the World Wide Web:

<http://nmrsgil.ncifcrf.gov/icmrbsxvii>

to provide updated information on the program as it is developed.

28th CONGRESS AMPERE on MAGNETIC RESONANCE, University of Kent, Canterbury, UK, September 1-7, 1996.

The meeting will be held at the University of Kent, located on a hillside overlooking Canterbury. The ancient city of Canterbury is famous throughout the world for its magnificent Cathedral. This beautiful building has played an important role in history and it contains the tombs of royalty, archbishops and cardinals. All accommodation and meals will be on the University Campus. The University of Kent is well served by road and rail from the major London airports, the south coast ports of Dover and Ramsgate and the Channel Tunnel. Given sufficient demand, arrangements will be made for coach travel to and from Heathrow and Gatwick airports.

A broad range of sessions will be tabled including the following topics:

- EPR, NMR, NQR and μ SR
- Defects and structures
- Diffusion and molecular motion
- Disordered and advanced materials
- Microimaging
- Modern developments in solid state NMR
- Multi-dimensional, quantum and resonance spectroscopy
- New Methods and approaches
- Non-equilibrium and non-linear phenomena
- Oriented systems
- Phase transitions
- Spin dynamics

A conference excursion, banquet and entertainment will be available together with a social program for accompanying guests.

The organising committee consists of Prof. J.H. Strange (Chairman), Dr. M.R. Halse (Secretary), Dr. M.E. Smith (Secretary), Dr. E.R.H. van Eck, Dr. P.C.L. Stephenson, Dr. P.J. MacDonald (Surrey), Dr. J.M. Baker (Oxford), Prof. Sir P. Mansfield (Nottingham), Prof. P. Morris (Nottingham) and Prof. E.F.W. Randall (Queen Mary, London).

All prospective participants are asked to pre-register by February 14, 1996. The first circular can be obtained by contacting The Secretariat, 28th Congress Ampere, The Physics Laboratory, University of Canterbury, Kent CT2 7NR, UK; ☎: 44-0-1227-823767; FAX: 44-0-1227-827558; e-mail: ampere@ukc.ac.uk

ELECTRON PARAMAGNETIC RESONANCE of RADICALS and METAL COMPLEXES, 2nd International Conference of the Polish EPR Association, Warsaw, Poland, September 9-13, 1996.

General Information: The 2nd International Conference will be held in Warsaw in the Parkowa Hotel (accommodations and conference center) and Uniwersytecki Hotel (accommodations) both on Belwederska Street, near Lazienki Park.

Scope & Topic of the Conference: A broad range of problems which can be solved or helped by the use of EPR spectroscopy; its application in such fields as chemistry, biochemistry; physics and bio-physics; studies on paramagnetic intermediates generated by radiolysis and photolysis; technical aspects and modern trends in EPR spectroscopy and related techniques.

The following scientists have so far agreed to present plenary lectures (or to attend the conference): A. Alberti (Italy), D. Beckert (Germany), M. Brustolon (Italy), F. Callens (Belgium), A.G. Davies (UK), F. Gerson (Switzerland), B.C. Gilbert (UK), D. Goldfarb (Israel), A. Jezierski (Poland), L. Kevan (USA), H. Kurreck (Germany), Ya.S. Lebedev (Russia), A. Lund (Sweden), K.A. McLauchlan (UK), A. Plonka (Poland), E. Reijerse (Netherlands), S. Schlick (USA), M.D. Sevilla (USA), J. Stankowski (Poland), M.C.R. Symons (UK).

The social program will include an excursion, a conference dinner, an opera performance or concert, and sightseeing around Warsaw's Old City.

The Organizing Committee consists of Prof. Andrzej

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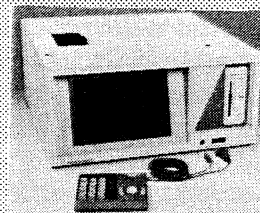
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For further information please contact Assoc. Prof. Hanna B. Ambroź, Inst. Nuclear Chemistry & Technology, ul. Dorodna 16, 03-195 Warsaw, Poland. ☎: 48-22-11-23-47, FAX: 48-22-11-15-32.

FIRST INTERNATIONAL SEMINAR ON SIMULATION MODELLING IN BIOENGINEERING (BIOSim 96), Merida, Venezuela, October 24-25, 1996.

The objective of this International Seminar is to bring together scientists who are carrying out research on the applications of computers to simulate biomedical problems. The Conference will be held at the Cultural Centre 'Tulio Febres Cordero', Merida. Conference topics will include:

- *Simulation of Physiological Processes*
- *Biomedicine*
- *Electrical and Magnetic Simulation*
- *Imaging Processing*
- *Data Acquisition and Analysis*

Inquiries and abstracts (by December 1, 1995 if possible) should be sent to Sue Owen, Conference Secretariat, BIOSim 96, Wessex Inst. Technology, Ashurst Lodge, Ashurst, Southampton, SO40 7AA, UK; ☎: 44-1703-293223; FAX: 44-1703-292853; E-mail: cmi@uk.ac.rl.ib; Intl. E-mail: cmi@ib.rl.ac.uk.

POSITIONS WANTED

EPR Spectroscopist seeks a Postdoctoral Fellowship. Solid state physicist/chemist, 26 years old, Ph.D. 1994 (physics and mathematics), researcher at the Institute of Chemical Physics (Moscow, Russia). Research experience: Investigation of the microwave response in HTSC, conducting polymers (polyaniline), synthesis of biradicals with the help of mechanoactivation. Please contact: Dr. D.S. Tipikin, Institute of Chemical Physics, Russian Academy of Science, Kosygin Str. 4, 117977 Moscow, Russia; ☎: 7-095-939-71-85; FAX: 7-095-938-21-56; E-mail: kinet@glas.apc.org.

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 biopolymers, 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 Postdoctoral Fellowship Position. Semiconductor physicist, 32 years old, Ph.D. '88, research scientist 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; E-mail: lab24@isph.nsk.su; ☎: 38-32-354255; FAX: 38-32-354265; Telex: 133243 FONON SU.

EQUIPMENT & SUPPLIES EXCHANGE

WANTED: EPR CAVITY

The Institute of Mineralogy, University of Marburg, Germany is looking for an EPR cavity for a Varian Model E-110 EPR, Q-band spectrometer. We would like to acquire a used cavity. If you have one available please contact Stefan Hafner, Inst. Mineralogy, Univ. Marburg, 35032 Marburg, Germany; FAX: 49-6421-288919; E-mail: hafner@mail.uni-marburg.de.

JEOL TE2000 SPECTROMETER

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

AVAILABLE: VARIAN MODEL EM-500 EPR SPECTROMETER

Acquired at a surplus sale: Varian Model EM-500 Spectrometer (Serial Number 500032A01); will trade for "anything" or, at worst, give it away. The device appears to be in good shape, weighs ca. 400 pounds, is an X-band Impact Diode device, and has a magnet with 4" diameter pole faces and 3/4" gap. If someone wants it they can pay for crating/shipping, or if local come get it with a small pickup truck. Varian has no records at all on this obsolete

machine. From its size and simplicity it appears to have been designed as a student teaching aid. The serial numbers on the electronic parts suggest that it was made somewhere about 1965. For more information, contact Albert Bauman, A.J. Bauman Associates, 524 Oakdale Drive, Sierra Madre, CA 91024-1429, USA; ☎: 1-818-355-8698.

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@du.edu; ☎: 1-303-871-2419.

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For more information contact Clarence Arnow, President. Voice: 708-677-4700; FAX: 708-677-0394
E-mail: mninco@wwa.com.

ANNOUNCEMENTS

MAILING LISTS FOR SCIENTIFIC MEETINGS

If you are planning a scientific conference, you may contact an officer of the International EPR Society or the IERC (address on front page of this Newsletter) to obtain a list of the 1,300+ Society members for use in issuing invitations. If you would like to have preprinted mailing labels, Martha Moore, who provides secretarial support for the Society, can do this at cost -- approximately \$50.00 (includes cost of labels, postage and, if you wish, a disk copy of the list in ASCII format). Labels for the entire database (3,800+ members and non-members) would cost approximately \$175.00.

1995 MEMBERSHIP DUES

Members: Have you paid your dues? If you are not sure, it will save the Society the expense of mailing late notices if you will take a moment to ascertain the status of your membership according to our records. To do this, please check the lower right hand corner of your mailing label. You will find there four dashes ("-- --"). If only the four dashes "-- --" or "--0--" appear, no dues have been recorded for you for the 1995 year. If dues have been paid, either a numeric value or the letter "R" or "C" (for soft currency countries) will appear, e.g. "--30--". If you don't have your label, please contact the IERC (address on page 1) and we will check to see if dues have been recorded. Your prompt payment of dues will be appreciated! For information on amount of dues and methods to pay, please see the IES World Wide Web home page.

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A full listing of regional treasurers of the IES and instructions for making payments may now be accessed via the World Wide Web. The address is:

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EPR NEWSLETTER

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Winter/Spring, 1996

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- Assistant Editor, Becky Gallivan, Urbana, IL (address below).
- Typography: Martha Moore.

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WWW: <http://ierc.scs.uiuc.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.

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

Welcome to the annual free public-distribution edition of the EPR Newsletter. If you are not a member of the International EPR (ESR) Society (IES) but enjoy reading this Newsletter, please join us in the Society!

Members get four issues a year and support several worthy activities. There are other members' benefits, too, such as greatly reduced subscription rates to the international journal *Applied Magnetic Resonance*; see Announcements on p. 28 for details. IES membership registration forms and instructions and other Society information appear in many Newsletter issues and in the Society's World Wide Web home page; the URL is: <http://ierc.scs.uiuc.edu/IES.html>. If you are a member but have not yet renewed your membership for 1996, please do so promptly. You may check the Treasurer's records to determine your payment status, through a link from the Society's Web site (see details on p. 28).

Corporate affiliates: We are delighted to welcome to the pages of the Newsletter two new IES corporate affiliates - CPI and Summit Technologies!

Reminder: Next January the IES Awards Committee will select 1997 awardees. Please, as soon as possible, do give the committees your suggestions. The "IES Affairs" column has information on submitting nominations.

Columns: Since our Newsletter specialty columns have been quite popular, several ideas have reached us suggesting others. In this issue, Hal Swartz, a recent winner of the IES Silver Medal in Biology/Medicine, initiates a "Biomedical EPR Corner" on a trial basis. He invites contributions for it and your reactions to it.

Congratulations: We salute the following winners of awards for EPR work: Brian M. Hoffman, 1996 Bruker Lecturer; Kev Salikhov, IES Gold Medalist; Jan Schmidt and Clyde Hutchison, 1995 Silver Medalists; Klaus Möbius, Johann-Martin Spaeth, and Ronald P. Mason, 1996 IES Silver Medalists; and Gunnar Jeschke, IES Young Investigator Awardee. See *Awards* in the "IES Affairs" column; also see "Notices of Meetings" section to find out about plans to present some of these awards. More extensive information about these awardees, their work, and the award events will appear in future issues of the Newsletter.

EPR Newsletter on the World Wide Web: The World Wide Web site URL for the EPR Newsletter is <http://ierc.scs.uiuc.edu/news.html>. This Web site is intended (1) to provide auxiliary material like program listings that are not printed in the Newsletter proper, (2) to provide advance information about content of upcoming issues, (3) to describe the Newsletters and how to obtain them, (4) to provide links to other relevant Web pages (e.g., those for EPR-related conferences), and (5) to post auxiliary announcements from the editorial offices. Please transmit your comments and suggestions regarding this site.

R. Linn Belford, Editor

◆ **IES AFFAIRS** ◆
ANNOUNCEMENTS AND
REPORTS FROM THE INTER-
NATIONAL EPR SOCIETY

From the President —

As I sit in Oxford writing this the sun is streaming through my windows and the first flowers of spring are breaking through after what has been an unusually hard winter. With experience of British weather I know that it will probably be terrible again tomorrow, but nevertheless spirits are lifting today and it is impossible not to be optimistic.

Running a Society such as ours always generates worries of its own. Will the members stay with us? Will our sponsors continue their magnificent support? Well, I am happy to tell you that the membership is once more increasing, and the number of sponsors is also increasing. All is not as well as it could be, however. Not unusually, some members simply forget to pay their subscriptions each year, which causes us cash-flow problems and effort reminding them. We should be grateful if prompt attention could be given to our yearly requests, and in particular if any remaining late payers this year could extract the sum from the sock underneath their bed (the traditional money storage of the British, which I do not recommend!) and send it to us.

It is also the case that our database contains many names who are no longer active in EPR/ESR, and misses many that are. We should be very grateful for any input from our members in helping us to up-date the list. This can be done very simply to the IERC using either letters or e-mail.

Finally, since the Society was formed, a whole generation of graduate students has flowed through our laboratories, but our membership has not increased as rapidly as we might hope. We should be grateful again if Research Directors could help in bringing the Society to the attention of their students (who may join whilst doing their doctorates at special student rates).

I have the advantage of working with a wonderful and industrious Committee, always making new suggestions to me, and always working on your behalf. But in the matter of membership there is only a certain amount we can do, and we need your help. I am immensely proud of what the Society has become, and it is successful by any international standards in the size of its membership. Nevertheless there are things we should like to do, particularly in the support of young scientists and in the support of conferences, which we are at present unable to. The Society does not yet have the income for this, and it must be our aim to rectify that.

I hope you all enjoy your personal Springs, whenever they may happen.

Keith McLauchlan

Awards —

Congratulations to the 1995 and 1996 Awardees. As we go to press, the following awards were announced by the respective Chairs of the International EPR(ESR) Society Awards Committees:

The 1996 IES Gold Medal in Physics/Instrumentation has been awarded to Prof. Kev Salikhov of the Russian Acad. Sciences, Kazan Physical-Technical Inst., Kazan, Russia.

The 1996 IES Silver Medal in Biology/Medicine has been awarded to Dr. Ronald P. Mason, NIH/NIEHS, Lab Molecular Biophysics, Research Triangle Park, NC, USA.

The 1996 IES Silver Medal in Chemistry has been awarded to Prof. Klaus Möbius, Free Univ. Berlin, Inst. Experimentalphysik, Berlin, Germany.

The 1996 IES Silver Medal in Physics/Instrumentation has been awarded to Prof. Johann-Martin Spaeth, Univ. Paderborn, Dept. Experimental Physik, Paderborn, Germany.

The Young Investigator Award goes to Gunnar Jeschke of Prof. Arthur Schweiger's group at ETH Zürich, Lab. Physical Chemistry, Zürich, Switzerland.

More details on the awardees and plans for presentation will be in later issues of the EPR Newsletter.

We also have been reminded that the 1995 Silver Medal Award for Physics/Instrumentation went to Prof. Jan Schmidt, Univ. Leiden, Huygens Lab, Leiden, Netherlands and the 1995 Silver Medal Award for Chemistry to Prof. Clyde Hutchison, Univ. Chicago, Dept. Chemistry, Chicago, IL. Details of the presentations of the awards will appear in a future issue.

The 1996 Bruker Award for EPR Research in Chemistry has been awarded to Prof. Brian Hoffman, Northwestern Univ., Dept. Chemistry, Evanston, IL. We repeat here the Society's award policies: Awards are not restricted to IES members, but the committees may take membership into account when deciding on the award winners. Agreement has been reached between the British and Russian Groups and ourselves to co-operate in the award of the Bruker and Zavoisky Prizes and our Gold Medal Award each year, with each group invited to make input into the selection of each, but with the final choice left to each group. The area of research interest is to rotate between the groups each year, with the loosely-interpreted categories, chemistry, physics and instrumentation, and biological sciences (including medicine). These categories are meant to be interpreted liberally and not to be restrictive.

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Fellows of the Society —

The IES has created Fellowships to recognise truly outstanding contributions and achievements in electron paramagnetic/spin resonance among these scientists (hopefully, IES members) who are either retired or are close to retirement. (Fellows of 1995: Anatole Abragam, Brebis Bleaney, Clyde Hutchison, Aleksandr Prokhorov and Samuel Weissman). The highest international standards are to be applied to the recognition of those worthy of this distinction, and their formal connection with the Society will enhance its own image. Nominations for consideration by the Committee are to be sent in confidence to Keith McLaughlan.

THE COMPUTER CORNER

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

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

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

Operating Systems and Cross-platform Considerations
 by Reef Morse

Most data acquisition systems are based on the PC platform, but more and more applications are using workstations (for example, the Sun, Silicon Graphics, DEC Alpha, and IBM RISC platforms). The price/performance ratio of these workstations makes it now feasible to use them for data acquisition as well as for data analysis.

However, for most applications, a simple PC will suffice. Most unmodified EPR spectrometers have response times of 100 msec; it makes no sense to collect data more quickly than that (10 kHz). This is well within the range of even an 8088 processor.

So, the question now becomes, what operating system to use? If you decide to run under Windows on a PC, then you

need a much more powerful computer just to run the operating system; the acquisition of data becomes almost incidental to the housekeeping of Windows. It is also much more difficult to write data acquisition software for a windowing environment. These factors are offset by the advantages gained in multitasking. For example, it is not uncommon for someone to be collecting data in one program, processing it in another, and plotting the data from a third, all while using a word processor, gathering electronic mail, and browsing the World Wide Web.

Windows-based data acquisition programs are available. Bruker bundles Windows-based software with their most recent line of relatively inexpensive EPR spectrometers. For the do-it-yourself types, LabView and LabWindows are good options. Scientific Software Services is developing a platform-independent data acquisition module and the software to run it under Windows. Dave Duling has Windows-based software available free-of-charge on his ftp/web site. Windowing operating systems are clearly the most attractive environments and more and more software should be available for satisfying the need to do many things at once. Should I buy it, write it myself, or have my research students do it?

These considerations are driven by time and money. If you have money and no time, it is easier to purchase a ready-to-run system. If you have time and no money, then you must write it yourself or have your research students do it. If you have a highly specialized system that no commercial vendor supports, then it also makes sense to develop your own software for your own lab.

Some other considerations are: 1) In general, the suppliers of ready-to-run software have been around for a while and can give you support. It often happens that EPR systems get taken over by someone unfamiliar with the software and it helps if they have a vendor to call. 2) In general, software and hardware developed by graduate students is not well documented and their interest in supporting the system diminishes as a step function when they leave. 3) Supporting and maintaining software, and developing improved versions of the software, is time-consuming (and therefore expensive). Vendors have a vested interest in satisfying their customers; graduate

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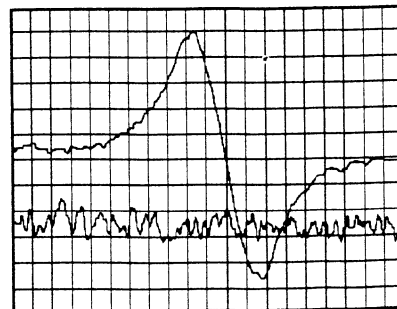
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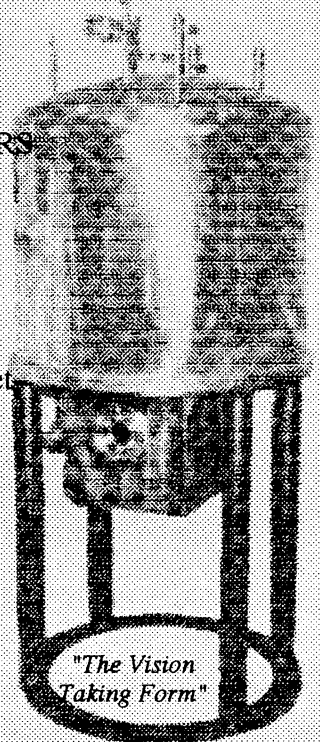
The plot illustrated was taken with a Varian weak pitch sample in a TE102 cavity under the conditions specified in the Varian E Line Series unmodified (E102/E108 bridge) instruction manual. Signal to noise ratio represented is 245:1. A 2.5 conversion factor was used to convert rms noise to P-P noise. The weak pitch sample had a .663 multiplication factor. Without the multiplication factor, the signal to noise would be 369:1.



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students have a vested interest in getting their degree and moving on. 4) The time that it takes to develop a system can be considerable. Sometimes there is no choice in this matter; the hardware you have may be so specialized that software must be developed and maintained in-house because of the prohibitive cost of hiring professional outside help. However, a good programmer can often solve a problem many times more quickly than you can yourself.

If you decide to undertake the development yourself (that is, in your laboratory), it is critical that all parties involved in the development understand the importance of adequate documentation. In the commercial field, good practice dictates three lines of comments for every line of code. Although most programmers balk at this restriction, it is important that the code be understandable by the next generation of students who will want to modify, improve upon, and/or fix, the existing software and hardware. Your only link between generations is the documentation and comment lines that clearly explain the intent of the code or the function of the hardware.

Reaching our World Wide Web and FTP sites:

The Illinois EPR Research Center has set up a Web page which will allow access to many other EPR Web pages. Point your browser at <http://ierc.scs.uiuc.edu> to access the IERC Web home page. Near the bottom, you will find a category "Other EPR Sites", under which is a self-explanatory list of links to other EPR WWW sites. Click on any line in this list to open the corresponding EPR

home page. Please E-mail the IERC (ierc@uiuc.edu) about EPR sites that should be added.

The IERC (ierc.scs.uiuc.edu) and Illinois State University (xenon.che.ilstu.edu), in cooperation, maintain anonymous ftp servers which include vendor demonstration programs (xenon), public domain software (ierc), and Rich Cammack's software data base.

BIOMEDICAL EPR CORNER

by
Hal Swartz

This is a trial at a possible regular feature for the Newsletter. It would provide updates on what is happening in this area of EPR applications and would be aimed at providing the general membership of the Society with a capsule view of "What's Hot and What's Not" in this exciting and relatively new area. Its success will depend on the interest and willingness of those in the field to contribute to this feature. Unless stopped by the editor or preempted by the receipt of contributions to this column from others, I will continue to write the column. (This is a not-so-subtle plea for others to contribute, with the accompanying threat of having to read my stuff if you don't!). The discussion "Why bother with *in vivo* EPR?" below is meant to be not only informative, but also thought-provoking about the kinds of contributions that you might consider making to this column.

We also could use this column for communications from any of us to others working in the area. As an illustration of this feature and also as a real use of this, I make the following request. Announcement to investigators using *in vivo* EPR (ESR): Please send me your complete list of publications pertinent to *in vivo* EPR, including papers in draft that you are willing to share. I have committed to a chapter on *in vivo* EPR for a book being edited by Larry Berliner, and I want it to be as inclusive as possible. Any material that has not yet been published formally will be appropriately referenced so as to insure its proper attribution and not preempt its eventual publication in the refereed literature. Please send the information by post (Hal Swartz, HB7252, Dartmouth Medical School, Hanover, NH, USA, 03755) or e-mail (harold.swartz@dartmouth.edu).

"Why Bother with *in Vivo* EPR?"

Despite a lot of activity recently on the development of capabilities to carry out *in vivo* EPR, it is not intuitively clear that this is such a great idea. There certainly are formidable technical problems (the subject of a future column), so there needs to be a strong biological rationale to make attacking these problems reasonable—especially as the likely solutions are unlikely to involve the kinds of fundamental physical problems that are intrinsically attractive to many physically oriented scientists.

To a biologist, the principal conceptual attraction of *in vivo* spectroscopy is the possibility of observing processes

under biologically and physiologically pertinent conditions. Some of the things I will say here could apply to any *in vivo* spectroscopy; the specific challenge is to discover where and how *in vivo* EPR can do this better or as well as other *in vivo* spectroscopies or when it is complementary to them.

Because of the immense complexity of animals, with the interactions of all of the different organ systems and all of the different types of cells within each organ system, many processes cannot be studied in model systems or in those at a lower level of organization such as cells isolated from the animal, isolated pieces of tissues, or even isolated organs. (And the latter also has many of the technical problems which make it so challenging to carry out true *in vivo* studies.) For example, the effects of anesthesia on the functioning of the cerebral cortex involves changes attributable not only to direct physical-chemical effects on the neurons, but also to those in the various excitatory nerves which affect function, in the flow of blood and the various nutrients within it, in the output of substances from other organs which directly or indirectly affect the functioning of the neurons, etc. Even for processes that appear to be analyzable at the cellular level, e.g., the formation of paramagnetic states of metal ions in the process of metabolism by cells, it is desirable to determine if these occur under the special conditions that may pertain *in vivo*. *In vivo* there can be associated phenomena such as the interactions of components of the blood, such as ascorbate. There may be potential artifactual effects from the environment in the cell culture system which do not occur in cells within their usual organs, because of the different surfaces, the composition of the medium, etc.

While these types of arguments, which led to the initial attempts at *in vivo* EPR, still are valid and very powerful motivations for continuing to explore this approach, much of the momentum for *in vivo* EPR development now comes from some of the specific types of parameters that have been found possible to measure with these techniques. The importance of making a particular measurement by *in vivo* EPR derives from (1) the ability of EPR to make the measurements uniquely or better than alternative methods and (2) the intrinsic biomedical significance of the parameter

that is being measured. Probably the most prevalent example, in my view, of a case that meets these tests is the measurement of the partial pressure or concentration of oxygen in living tissues. The effects of oxygen on EPR spectra are an old story to EPR spectroscopists, and this phenomenon has been widely exploited to make measurements in model systems and in cells. The method works well *in vivo* also, especially because of the development of oxygen-sensitive paramagnetic materials which are both very responsive to the partial pressure of oxygen and also very stable and nonreactive. Consequently, once they are placed into tissues they provide an essentially unique capability to make repeated accurate non-invasive measurements of the partial pressure of oxygen from a known site in tissues *in vivo*. This capability has a wide range of experimental applications because of the importance of oxygen in both physiological (normal) and pathological (diseased) processes. EPR also appears to provide a unique capability to follow reactive species *in vivo* when these have unpaired electrons (i.e., free radicals and the states of some paramagnetic metal ions whose spectra can be resolved at physiological temperatures). A variety of other biological and pharmacological phenomena now also seem to be amenable to study by EPR *in vivo*, in which the information obtained has potentially high biomedical value. These include physical-chemical parameters such as pH and motion, redox activity (especially by following the redox metabolism of nitroxides), the use of a paramagnetic reporter as a tracer of a labeled molecule, and measuring radiation doses. The list of potentially valuable applications continues to grow as more is learned about how to carry out *in vivo* EPR and more people become involved in this field.

Another related aspect which seems to be a driving force for developing *in vivo* EPR is the possibility of carrying out such studies in humans. Areas in which *in vivo* EPR appears to have a potential to provide a valuable addition to medical capabilities include following the partial pressure of oxygen in tissues (e.g., monitoring the state and response to therapy of peripheral vascular disease), following the metabolism and distribution of drugs that are spin labeled or have free radical intermediates, and, eventually, using the whole range

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of capabilities noted above for experimental studies where such measurements could have an impact on understanding and/or treating disease in patients.

So in summary, the main reason to continue development of *in vivo* EPR is that it already has demonstrated the potential to provide valuable biomedical information that, I submit, cannot be obtained as well by other techniques. Results at this relatively early stage of development suggest that it will continue to grow in extent and importance for a considerable time. BUT there are some formidable practical obstacles to carrying out such studies. These will be discussed in a subsequent column.

EPR SPECIALIST VIGNETTES

Edited by
Arthur Schweiger

Optically Detected Magnetic Resonance (ODMR) of Triplet States

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Introduction

Optical detection of magnetic resonance (ODMR) is often advantageous because it pairs the frequency resolution of magnetic resonance with the sensitivity of optical spectroscopy. Resonant transfer of population between the three triplet sublevels generally gives rise to a concomitant change in the optical properties (phosphorescence, fluorescence, absorption) of the sample, because of the different decay characteristics of each sublevel. It is preferentially carried out in zero magnetic field, where the triplet wave functions are not mixed by the Zeeman interaction and the triplet sublevels are split by the dipolar interaction between the two unpaired electrons (and to a lesser extent by electron - nuclear hyperfine interactions with nuclei of $I \geq 1$). This enhances considerably the resolution

and sensitivity for disordered systems. A further advantage is that the modes of detection and excitation are decoupled, so that one is insensitive to noise sources due to the microwaves (as e.g. amplitude fluctuation), especially when the transition is saturated. (Note that the optical signal does not disappear upon saturation as does the microwave absorption in microwave detection; this is another advantage of optical detection.)

The principal results of an ODMR experiment are: 1) proof of the photoproduction of one or more triplet states, 2) the determination of highly accurate values of the zero-field splitting (ZFS) parameters, 3) the determination of the individual sublevel molecular decay rates and populating probabilities, 4) information on environmental interactions through line shape analysis and hole-burning, 5) spectral information via optical-microwave double resonance experiments, 6) with LD-(T - S) spectroscopy detailed information on the orientation of the triplet spin axes and on relative angles of singlet transition moments may be derived.

The ZFS parameters and the sublevel populating probabilities and decay rates are fingerprints of molecular structure. They are also sensitive to environmental effects, which in addition to line shape analysis and hole-burning allows one to use the triplet state as a probe of secondary and tertiary structure, e.g. of proteins and nucleic acids and their complexes, and of pigment environment in photo-synthetic structures.

Keeping the microwave frequency constant at one of the resonant values (there are generally three ODMR resonances corresponding to the three ways one can connect two out of three triplet sublevels with resonant microwaves), one can scan the wavelength at which the resonance is detected. This gives the microwave-induced phosphorescence, fluorescence or absorption spectrum. The latter corresponds to the optical triplet - singlet (T - S) difference spectrum, which in principle carries much information, especially when the triplet-containing molecule interacts with other chromophores in its environment. In this Vignette the physical background of ODMR will be sketched briefly, followed by a few highlights of its application in biology and biochemistry. More information can be found in reviews by Maki (1984) and Hoff (1989,1990,1993).

The triplet spin Hamiltonian in zero magnetic field

The triplet spin Hamiltonian without external magnetic field comprises interactions involving the magnetic moment of the electrons. The main contribution to the spin-spin coupling operator, \hat{H}_{SS} , is the classical magnetic dipole-dipole interaction between two electrons, \underline{D} , a tensor operator whose elements consist of integrals over the coordinates of the electrons,

$$\hat{H}_{SS} = \hat{S} \underline{D} \hat{S} = -X \hat{S}_x^2 - Y \hat{S}_y^2 - Z \hat{S}_z^2 \quad (1)$$

where \hat{S} is the total spin angular momentum operator $\hat{S} = \hat{s}_1 + \hat{s}_2$, with \underline{s}_1 , \underline{s}_2 the magnetic moments of the two electrons. X, Y and Z are the principal values of \underline{D} , and \hat{S}_u

($u = x, y, z$) the components of \hat{S} along the principal axes of \hat{D} . Often, these axes coincide with the molecular symmetry axes. The triplet spin functions $|T_u\rangle$ ($u = x, y, z$) are eigenfunctions of \hat{H}_{SS} with the property

$$\hat{S}_u|T_u\rangle = 0, \quad \hat{S}_x|T_y\rangle = -\hat{S}_y|T_x\rangle = |T_z\rangle \text{ (cyclic)}. \quad (2)$$

Thus, there is no net magnetic dipole moment associated with any of the triplet substates in zero magnetic field, $\gamma\hbar \langle T_u | \hat{S} | T_u \rangle = 0$, but there is a transition dipole moment present between any two of the triplet substates, $\gamma\hbar \langle T_x | \hat{S}_y | T_z \rangle = i\gamma\hbar$ (cyclic), where γ is the gyromagnetic ratio of the electron and \hbar is Planck's constant divided by 2π . Thus, in zero magnetic field, population can be transferred from one triplet sublevel to another by applying a resonant electromagnetic field. It follows that the transition probability is proportional to

$$|\gamma\hbar \langle T_z | \hat{B}_1 \cdot \hat{S} | T_y \rangle|^2 = (\gamma\hbar B_{1x})^2 \text{ (cyclic)} \quad (3)$$

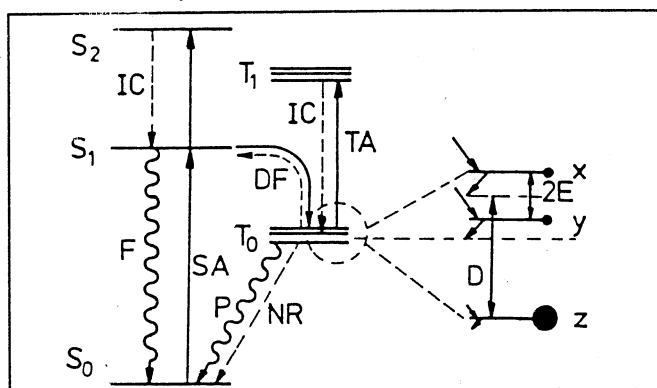


Figure 1: Energy level diagram of the singlet and triplet manifold. S_0 , singlet ground state; S_1 and S_2 , singlet excited states; T_0 and T_1 , first and second excited triplet states; SA and TA , singlet and triplet absorption, respectively; F and DF , fluorescence and delayed fluorescence, respectively; P , phosphorescence; NR , non-radiative transition; IC , internal conversion. Enlarged T_0 levels: X , Y and Z , eigenenergies of the dipole-dipole interaction; D and E , zero-field splitting parameters. Downward arrows to the right, populating probabilities; to the left, decay rates; filled circles, equilibrium populations. From Hoff (1989).

where \hat{B}_1 is the amplitude of the magnetic component of the driving field, $\hat{B} = \hat{B}_1 \cos \omega t$. From Eqn. 3 it follows that the microwave transition $T_u \approx T_s$ ($u, s = x, y, z$) is polarized with transition moment along $\underline{w} = \underline{u} \times \underline{s}$. This property allows us to perform microwave-selection spectroscopy, to which we

will turn later.

The resonance frequencies follow from the eigenenergies of \hat{H}_{SS} , viz. X , Y and Z (Fig. 1). Because $X + Y + Z = 0$ (the trace of \hat{D} is zero), it is customary to express the energies in two independent parameters D and E , the ZFS parameters:

$$D = -\frac{3}{2}Z, \quad E = -\frac{1}{2}(X - Y) \quad (4)$$

with by convention $|D| \geq 3|E|$. The zero-field splitting parameters represent averages over the spatial coordinates x' , y' , z' of the distance vector \underline{r} of the two unpaired electrons, E being a measure of the deviation from axial symmetry about the Z -axis. The relative order of the energy levels depends on the sign of D and E . For a flat molecule such as an aromatic amino acid residue, or a chlorophyll, one would expect D to be positive. (The z -axis is the axial symmetry axis and is perpendicular to the plane of the molecule, so that the z' component of \underline{r} is on average much smaller than $|\underline{r}|$, making $Z < 0$.) For a rod-like molecule, such as a bi-radical, D will be negative.

Optical detection of magnetic resonance, ODMR

Principles. Continuous illumination will generate an equilibrium population of the triplet sublevels, given for light levels that are not too high by

$$N_u = p_u KN/k_u, \quad \sum_u N_u = N_T, \quad u = x, y, z. \quad (5)$$

p_u is the probability to transit from the singlet excited state to the u -th triplet sublevel with $\sum_u p_u = 1$, k_u the decay rate that governs de-excitation from the u -th sublevel back to the singlet ground state, K the overall rate of populating the triplet state, N_u the population of its u -th sublevel, N_T its total population and N the number of photoexcitable molecules. Both p_u and k_u are determined by molecular symmetry. When a microwave field is switched on, for example of a frequency corresponding to a transition between the y - and the z -level, the field will transfer population between these two levels, and a new equilibrium will be established that for a strong enough microwave field is given by $N'_y = N'_z = p'KN/k'$ with $p' = \frac{1}{2}(p_y + p_z)$ and $k' = \frac{1}{2}(k_y + k_z)$. If we take $p_y \approx p_z$ and $k_z \ll k_y$, then it is

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seen immediately that $(N'_y + N'_z) < (N_y + N_z)$, because for $k_y > k_z$, $2/(k_y + k_z) < 1/k_y + 1/k_z$. The x-level will sense the new equilibrium via the photogeneration cycle of the triplet state, but this is a small second order effect. The change in triplet population will lead to a change in phosphorescence or fluorescence intensity, or in the singlet ground state absorbance. For saturating microwaves the change is given by

$$\Delta N_T = (k_u - k_v)(N_u - N_v) / (k_u + k_v) \quad u, v = x, y, z \quad (6)$$

In the above we have the essence of ODMR. A sample is continuously illuminated at liquid helium temperatures, preferably below 2.1 K for inhibiting spin-lattice relaxation, and simultaneously irradiated by microwaves of a frequency ν not far from that corresponding to one of the triplet sublevel spacings: $\nu_{1,2} = (|D| \pm |E|)/h$ and $\nu_3 = 2E/h$ (Fig. 1). The frequency ν is slowly scanned across one of the frequencies $\nu_{1,2,3}$ while either the phosphorescence, (delayed) fluorescence or absorbance of the sample is monitored. When ν is close to or precisely equal to $\nu_{1,2,3}$ the ensemble of triplet state is in resonance with the microwave

field and the fluorescence (FDMR), phosphorescence (PDMR) or absorbance (ADMR) will be enhanced, or diminished, depending on the relative values of p_u and k_u . Note that the FDMR or ADMR signal intensity is proportional to ΔN_T , and therefore to the *square* of the incident light intensity, because one photon is used for producing the triplet state and a second for probing the microwave-induced change in the optical parameter.

Time-resolved ODMR. The time dependence of the ODMR signal in response to a change in the condition of microwave irradiation (switching them on or off, or applying pulses) is given by the solution of the differential equations describing the time development of the four-level system S_0 , $T_{x,y,z}$, simplified by the neglect of the S_1 population. The general analytic solution is given by Hoff and Cornelissen (1982); for the present discussion it suffices to note that the response of the system to switching on or off resonant microwaves connecting $x \approx z$ or $y \approx z$ or both is given by the sum of three exponentials. Special cases are:

a) For light flux $K \rightarrow 0$, spin-lattice relaxation $W \approx 0$ and in the absence of microwaves, the triplet sublevels are

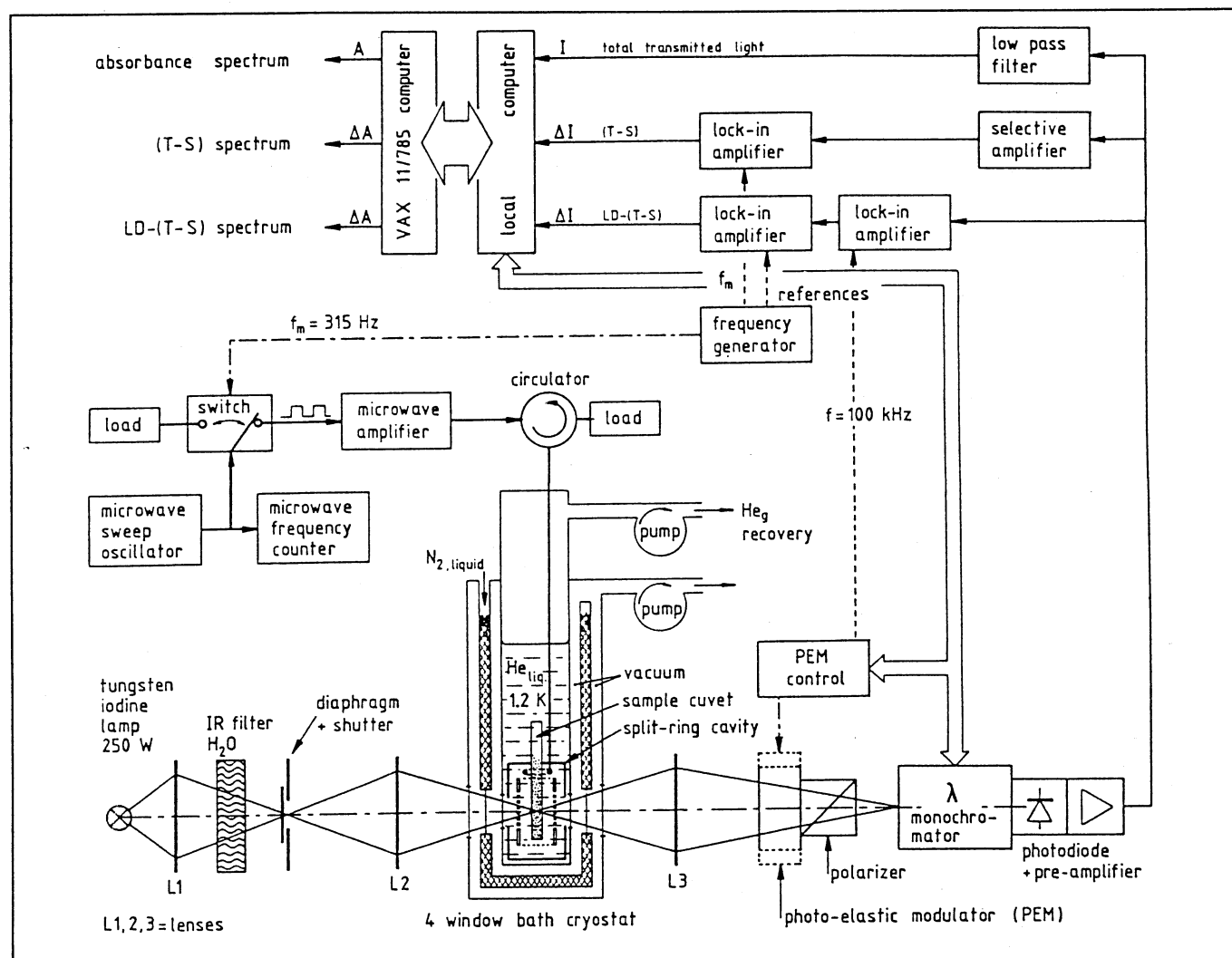


Figure 2a: Block scheme of the ADMR and LD-ADMR set-up. From Lous (1988).

uncoupled. After some perturbation each sublevel decays according to

$$N_u(t) = N_u(\infty) - [N_u(\infty) - N_u(0)]\exp(-k_u(t)). \quad (7)$$

b) For brief microwave pulses resonant between two triplet sublevels, u and v , and for $K \rightarrow 0$, $W \approx 0$, the return to equilibrium is described to a good approximation by two exponentials with characteristic rates given by

$$\lambda_{1,2}(K) = -k_{u,v} - p_{u,v}K \quad K \rightarrow 0; u \neq v = x, y \text{ or } z \quad (8)$$

and with amplitudes of opposite sign. Provided K is low enough, the third sublevel is not perturbed.

c) When saturating microwaves are applied simultaneously to two of the three ODMR transitions, the triplet collapses to one level with average decay rate $k = 1/3 \sum_u k_u$. The set of differential equations describing the simplified four-level system then reduces to those for an equilibrium reaction, which immediately yields

$$N_T(t) = NK(K + k)^{-1}[1 - \exp(-(K + k)t)] \quad (9)$$

for the triplet built-up after the onset of illumination at $t = 0$. Eqn. 9 permits the evaluation of k by extrapolation to $K \rightarrow 0$. Obviously, the same equation applies when the triplet levels are coupled not by microwaves but by spin-lattice relaxation at higher temperatures. In fact, the latter method to determine k is to be preferred, since especially for randomly-oriented samples the condition of microwave saturation is difficult to obtain.

Double resonance

Optical. Once the ODMR lines of a triplet have been determined, the resonance frequencies are known precisely, and one can investigate the dependence of the intensity of a particular resonance line on the probing wavelength. The resulting spectra may be called microwave-induced phosphorescence, fluorescence or absorbance spectra, abbreviated by MIP, MIF and MIA spectra, respectively. For one particular triplet state, the shape of these spectra does not depend on the selection of the resonance frequency, i.e. ν_1 , ν_2 or ν_3 . Obviously, if more than one triplet state is present, for example in aggregates, the MI spectra provide

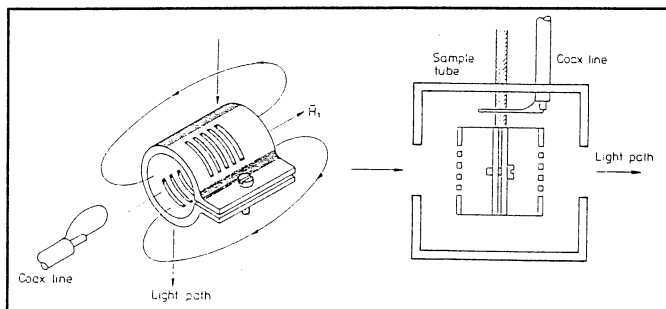


Figure 2b: Loop-gap resonator used for LD-ADMR experiments. The cavity resonance frequency is tuned by the screw governing the width of the gap. The B_1 field is along the cavity's cylinder axis. Dimensions: inner diameter, 20 mm; height, 60 mm. From den Blanken et al. (1984).

another means to sort out which resonances belong to the same triplet state. Conversely, MI spectroscopy allows the unraveling of complex optical spectra.

MIA spectra are a case apart, since they provide much more information than the MIP or MIF spectra. They represent the difference of the singlet ground state, 'normal', absorbance spectrum and the spectrum for the system when a triplet state is present (Fig. 3). By analogy to difference spectra obtained by optical flash spectroscopy, they have therefore been labeled triplet-minus-singlet absorbance difference (T - S) spectra (den Blanken and Hoff, 1982). Normally, the T - S spectrum is recorded with a single-beam optical spectrometer and the ADMR signal ΔI is normalized by the intensity of the incident light, I . It can be shown that for small ΔI the normalized change in transmitted light intensity is proportional to the change in absorbance ΔA . As mentioned above, $\Delta I \propto I^2$, so that for non-saturating light intensities, the amplitude of the T - S spectrum is proportional to I .

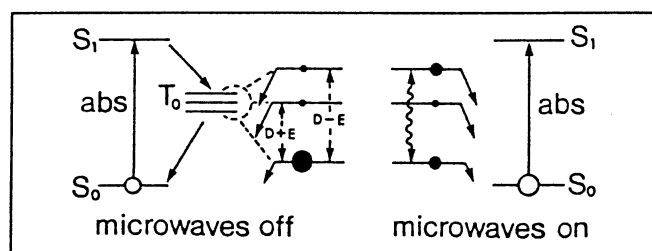


Figure 3: Principle of absorbance-detected magnetic resonance. Filled circles denote relative equilibrium population of the triplet sublevels, open circles that of the ground state. A saturating microwave field connecting two triplet sublevels (corrugated arrow) leads to a new (here higher) equilibrium value of the singlet ground state population, hence to a change in the absorbance. The same principle holds for fluorescence detection, while the phosphorescence is also enhanced by the microwave field. From Hoff (1989).

Microwaves. In another form of double resonance the sample is irradiated with microwaves of two different frequencies, one kept constant at a particular resonance line and one scanned over a certain frequency interval. There are two varieties of such a double-resonance experiment: either the microwaves of variable frequency or those at fixed frequency are amplitude-modulated. If in the first case the microwaves are scanned over the resonance excited by the fixed frequency, then one observes the resonance line with a "hole", centered at the "burn" frequency. Such a hole indicates that the resonance line is inhomogeneously broadened; its width recorded for low microwave power and narrow-banded excitation and probing, is twice the homogeneous width of the individual resonances making up the broad line. Alternatively, one may scan a different resonance, for example the $2E/h$ line. Burning at one of the $(|D| \pm |E|)/h$ transitions transfers population from the z -level to either the x - or the y -sublevel, so that their population

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difference is considerably enhanced and the $2E/h$ line becomes easily observable as an "anti-hole" (Hoff, 1976).

In the second case, the normal resonance line is not observed, and only the hole shows up having a baseline at the intensity level of the ADMR signal corresponding to the modulated microwaves, dipping to a level close to zero intensity when the frequencies of burn and probe microwaves coincide. This mode makes it somewhat easier to study variations in line shape as a function of burn power, etc. Both methods of carrying out a microwave double-resonance experiment are useful for assigning ODMR lines to a particular triplet state when several triplets contribute to the ODMR spectrum. If one of the lines is 'tickled' with microwaves, then from all other lines only those will be affected that represent either transitions within the triplet sublevel manifold to which the 'tickled' line belongs or which are due to a triplet whose concentration depends on that of the triplet that is 'tickled', e.g. because it is populated through triplet energy transfer from the latter triplet state. Note that, because the effects measured are usually very small, adequate care must be taken that interference of the two microwave channels is avoided. One precaution is to insert directional couplers or circulators in the two channels (Fig. 2a).

Linear dichroic T - S spectroscopy

The microwave transitions between the u and v triplet sublevels are polarized along $\underline{w} = \underline{u} \times \underline{v}$. This is analogous to an optical transition, whose transition dipole moment usually has a well-defined direction in the molecular frame. Unfortunately, often the position of the triplet axes, and therefore the directions of the triplet magnetic resonance transition moments, in the molecular frame of molecules of low symmetry is not, or not accurately, known. As will be shown below, LD-(T - S) spectroscopy provides a unique means to ascertain the directions of the magnetic transition moments. With this knowledge one may then derive from the LD-(T - S) spectra precise structural information on molecular aggregates.

In optical spectroscopy, the transition probability for a transition with transition dipole \underline{p} is proportional to $|\underline{E}|^2 |\underline{p}|^2 \cos^2 \beta$, where β is the angle between \underline{p} and the \underline{E} electric vector of the (polarized) incident light. A similar

relation holds for the magnetic microwave transitions between the triplet sublevels. Thus, for a microwave transition moment $\underline{\mu}_{mw}$ and an angle β between $\underline{\mu}_{mw}$ and the \underline{B} magnetic vector of the (polarized) microwave field, we have a transition probability $|\underline{B}_1|^2 |\underline{\mu}_{mw}|^2 \cos^2 \beta$. It follows that molecules oriented with $\underline{\mu}_{mw}$ more or less parallel to \underline{B}_1 have a much higher transition probability than those oriented about perpendicular to \underline{B}_1 . (Of course, for $\beta = 90^\circ$, the transition probability is exactly zero.) Hence, for random excitation to the triplet state, molecules oriented in an angular interval $d\beta$ close to $\beta = 0$ will experience a much higher change in their relative triplet concentration upon the application of (polarized) resonant microwaves than molecules in an interval $d\beta$ close to $\beta = 90^\circ$. Consequently, the distribution of triplet states, which was isotropic before the application of the microwaves, becomes *axially anisotropic* with the axis parallel to \underline{B}_1 when resonant microwaves are switched on.

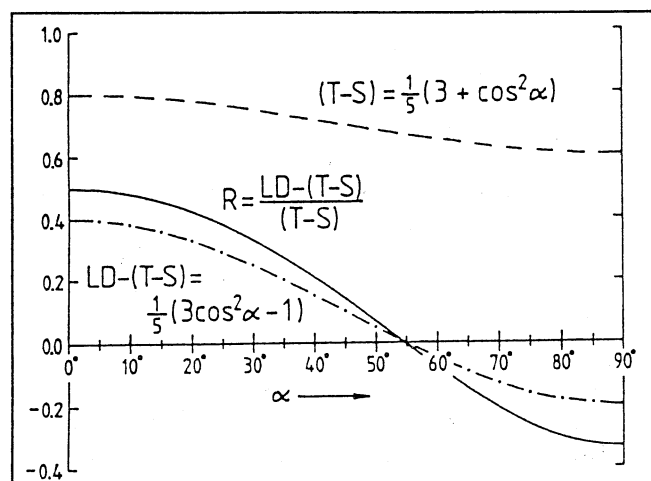


Figure 4: The dependence of the amplitude of the ADMR-monitored T - S and LD-(T - S) spectra and their ratio R on the angle α between the optical and the microwave transition moment. $\alpha = 54.7$ is the magic angle for which the microwave-induced linear dichroism is zero ($R = 0$). From Lous (1988).

Microwave-induced selection in the triplet state distribution is very similar to that of *photoselection*. We can therefore partake of the formalism derived for that technique (see e.g. Hoff 1985) to calculate the functional relationship between ΔA and α , the angle between \underline{p} and $\underline{\mu}_{mw}$. It can be shown that the ratio R of the intensity of the LD-(T - S) spectrum (which represents the difference $A_{\parallel} - A_{\perp} = (T - S)_{\parallel} - (T - S)_{\perp}$) and the T - S spectrum is given by

$$R = \frac{\text{LD}-(T - S)}{T - S} = \frac{3 \cos^2 \alpha - 1}{\cos^2 \alpha + 3} \quad (11)$$

Eqn. 11 is plotted in Fig. 4, together with plots of the LD-(T - S) and T - S intensities versus α . It is seen that R is quite sensitive to α , so that with proper calibration of the T - S and LD-(T - S) spectra, α can be determined quite

accurately. Of course, all this applies rigorously only for single absorbance bands. If bands with different directions of \underline{p} vis-à-vis $\underline{\mu}_{mw}$ overlap, R will have some intermediate value and one will have to simulate the complete LD-(T - S) and T - S spectra to obtain values for the various α 's.

The angle α in Eqn. 11 refers to one particular $\underline{\mu}_{mw}$, say that corresponding to the \underline{x} polarized $y \approx z$ transition at frequency $(|D| - |E|)/h$. Tuning the microwaves to the $(|D| + |E|)/h$ frequency, that is the $x \approx z$ or y polarized transition, allows the recording of LD-(T - S) spectra and the determination of R for a different α , viz. the angle α_y between \underline{p} and \underline{y} . When \underline{p} , \underline{x} and \underline{y} lie in one plane, $\alpha_y = 90^\circ - \alpha_x$, since the triplet spin axes \underline{x} , \underline{y} and \underline{z} span a Cartesian coordinate frame. If \underline{p} , \underline{x} and \underline{y} are not coplanar, the two measurements uniquely define the orientation of \underline{p} in the $\underline{x}, \underline{y}, \underline{z}$ coordinate frame. This is a great advantage over the ordinary photoselection experiment, where one determines just one angle between two transition moments, which leaves one with a conical ambiguity. Note that it suffices to record LD-(T - S) spectra for just two of the three possible ADMR transition frequencies.

Instrumentation

The minimal requirements for an ODMR experiment are a source of light, one of microwaves, a cryostat (preferably a double-walled helium bath cryostat equipped with at least two windows) and a detector. Up-to-date discussions of these parts and the relevant electronics are given by Maki (1984) and Hoff (1989,1990,1993). Here we will limit ourselves to a few notes and a discussion of special arrangements for ADMR and linear-dichroic (LD)-ADMR. A schematic diagram of our present ADMR set-up is shown in Fig. 2a. With small modifications it can be used for PDMR and FDMR as well.

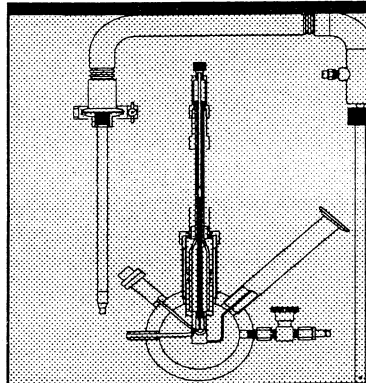
Crucial for high-sensitivity ADMR is a high-intensity, low-noise light source. To this end the high-power tungsten-halogen lamp powered by a current-stabilized DC power supply, introduced by den Blanken et al. (1982), proved very suitable, and is now an essential part of all ADMR spectrometers. Adequate filtering of infra-red radiation should be provided to avoid heating of the sample. When the excitation beam is broad-banded, it may also serve as probe beam at various wavelengths.

Microwaves are supplied preferably by a sweep unit (for example with a range of 0.1 - 27 GHz) with provisions to scan the frequency over the desired range and to amplitude- or frequency-modulate the output. Usually, the output (20 - 40 mW) is enough for regular ODMR at liquid helium temperatures without amplification. For measuring the ODMR lines the microwaves are fed into a broad-band resonator, e.g. a helix, that can admit the frequency range of interest. If one is interested in the (probe) wavelength dependence in MI spectroscopy, the microwave frequency is set exactly at resonance and a narrow-band cavity may be used. We have used a loop-gap resonator (Hardy and Whitehead, 1981) with slots for optical access (Fig. 2b). It provides a well-polarized microwave field, of which good use is made in LD-ADMR (see below).

The optical detector depends on the optical mode. For phosphorescence and fluorescence a photomultiplier is used. For ADMR, one may employ a strong probe beam (in fact the excitation beam may serve as such), providing a number of transmitted quanta that is sufficiently high for the use of a photodiode may be used (up to 1100 nm, silicon; 1100 nm - 2 μ m, germanium). To observe the resonance by fluorescence or phosphorescence, the wavelength of detection should be separated from the wavelength of excitation by adequate filtering. For ADMR, either a filter or, when the probe wavelength dependence is monitored, a monochromator is used.

The sensitivity of the ODMR spectrometer for slow-passage experiments can be considerably enhanced by modulating the amplitude of the microwaves and applying frequency-selective amplification of the photodetector signal combined with lock-in detection. For example, in our ADMR spectrometer a $\Delta A/A$ ratio of better than 5×10^{-7} is routinely achieved. Obviously, the modulating frequency has to be less than the slowest sublevel decay rate. For slowly decaying triplets ($k < 10 \text{ s}^{-1}$), one may be better off by scanning the line with unmodulated microwaves and employing signal averaging. For kinetic measurements broad-banded amplification of the detector signal and signal averaging are used.

Finally, as in all modern spectrometers the instrument is interfaced to a small, dedicated computer that handles



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monochromator setting, data collection and storage, and carries out simple operations as taking the $\Delta I/I$ ratio (important when recording the probe wavelength dependence).

LD-(T - S) spectroscopy. For LD-(T - S) spectroscopy we need polarized microwaves, therefore a simple helix is not suitable. We use the loop-gap cavity depicted in Fig. 2b. The B_1 field is polarized along the vertical, therefore it is perpendicular to the horizontal light beam. The probe light is unpolarized. The B_1 field induces in the transmitted light T an ellipticity ($\equiv T_{//} - T_{\perp}$), which is detected via a photoelastic modulator (PEM) after the sample, followed by a polarizer. The PEM rotates the ellipse spanned by the unequally-transmitted light vectors $E_{//}$ and E_{\perp} (with respect to B_1) by 180° at a frequency of 50 kHz. The analyzer converts this polarization modulation into an amplitude modulation at 100 kHz that is proportional to $T_{//} - T_{\perp} \approx A_{//} - A_{\perp}$ (T, transmission; A, absorbance) for small differences. The microwaves are as in T - S spectroscopy modulated at low frequency (say 315 Hz), so that the light intensity falling on the photodiode is doubly modulated at 100 kHz and 315 Hz. Demodulation at 315 Hz combined with suitable electronic filtering gives the normal T - S signal. Double demodulation at 100 kHz and 315 Hz gives the $(T - S)_{//} - (T - S)_{\perp} \equiv$ LD-(T - S) difference signal. The signal-to-noise ratio is enhanced by inserting selective amplifiers in both modulation channels. Scanning the monochromator yields simultaneously the T - S and the LD-(T - S) spectra. As before, the signals are divided by the intensity I to correct for changes in lamp output, monochromator sensitivity, etc. as a function of wavelength. To correctly evaluate the ratio R (Eqn. 11) one must mutually calibrate the T - S and LD-(T - S) signals, e.g. by simulating the transmitted modulated light by a modulated light-emitting diode (LED). Care has to be taken to avoid as much as possible ellipticities induced by extraneous sources, such as the lamp, cryostat windows, sample cell, etc. In our set-up these extraneous ellipticities amounted to less than 1% of the LD-(T - S) signal.

Applications of ODMR in biology

ODMR in proteins. All proteins contain naturally-occurring triplet probes, namely their aromatic amino acids: phenylalanine (phe), tryptophane (trp) and tyrosine (tyr).

Histidine does not show an observable triplet state, whereas phe is firstly difficult to excite, and secondly it loses the excitation easily by energy transfer, so that in practically all applications of ODMR in protein research, mostly in the groups of Kwiram and Maki (reviewed in Maki, 1984, and Hoff, 1989, 1993) attention was focused on the study of the triplet states of tryptophanes and tyrosines in vitro and in various proteins using phosphorescence for the detection of the magnetic resonance. Often, in proteins that contain several trp and/or tyr, energy transfer occurs to the aromatic residue with lowest energy, so that only one trp or tyr is observed. In some cases, however, the individual aromatic residues could be distinguished, for example trp and tyr in azurin, trp's in bovine serum albumin and in lysozyme and tyr's in triply point-mutated lysozyme of the bacteriophage T_4 , which contains no trp.

Aromatic residues close to active sites of enzymes are expected to be sensitive to substrate or dye binding. Triplet-singlet energy transfer may occur, e.g. from trp to proflavin bound to chymotrypsin, which allows detection of ODMR resonances of trp via the delayed fluorescence of proflavin, or triplet-triplet transfer between substrate or dye and aromatic residue. Also signals from coenzymes, such as NAD^+ and NADH, are readily observed by ODMR and give information on the conformation of the cofactor in the enzyme.

The triplet yield can be appreciably enhanced by complexing a closed-shell heavy metal component such as Ag^+ or methyl mercury (II) (CH_3Hg^+) to aromatic residues (Bell and Brenner, 1982; Zang et al., 1989). Because of the large nuclear mass (Z number) of e.g. mercury, spin-orbit interaction and therefore the intersystem crossing efficiency is dramatically enhanced. Orbital overlap between the aromatic residue or nucleic acid base and the metal compound provides the required interaction, which is spin-sublevel selective (Gosh et al., 1987, 1988). Subtle changes in the binding of the heavy-metal component, for example induced by protein conformational changes, may give rise to large changes in the populating probabilities and the decay rates of the individual triplet sublevels.

ODMR in photosynthesis. The use of ODMR in photosynthesis research has proved to be a particularly fruitful field of its application in biology. By far the most important

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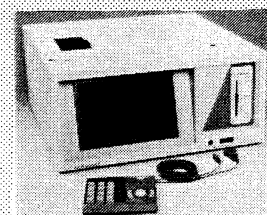
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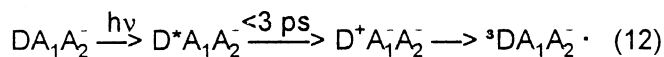
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triplet state in photosynthetic membranes is that generated on the primary electron donor by radical recombination under conditions that forward electron transport is blocked by the prereduction of one of the acceptors (or by its physical deletion):



Reaction (12) takes place in the so-called reaction center (RC), a specialized pigment-protein complex. The structure of two bacterial RC has been elucidated in atomic detail by X-ray crystallography (Deisenhofer et al., 1985; Chang et al., 1986; Allen et al., 1987, Ermler et al., 1994). D is a bacteriochlorophyll (BChl) dimer, A_1 is a bacterio-*pheophytin* (Φ_A), A_2 is a quinone, Q_A . There are another Φ molecule, Φ_B , and two so-called accessory BChls (B_B and B_A) whose function is still under debate. The pigments subscripted with A and those subscripted with B are arranged in two chains that show C_2 symmetry with D on the symmetry axis.

Because A_2 is prerduced and cannot normally accept two electrons, the radical pair $D^+A_1^-$ recombines in about 20 to 50 ns to either the singlet excited or ground state of D, or with almost 100 % yield at cryogenic temperatures to its triplet state, 3D (Dutton et al., 1972).

Applications of ODMR have included fluorescence detection (reviewed in Hoff, 1982, 1989) and absorbance detection. Because the latter technique now dominates the field we will mostly discuss applications of ADMR to various photosynthetic preparations.

ADMR spectroscopy of reaction centers. The great advantage of the ADMR variant above fluorescence or phosphorescence detection is that it can always be applied, regardless of quantum yields of emission, provided the lifetime of the triplet state is not too short (this holds for all cw ODMR techniques) and a sufficient optical density can be attained ($OD \approx 0.7$ gives maximal signal). Both conditions hold for the photosynthetic triplets, and in the first application of ADMR to isolated bacterial RCs (den Blanken et al., 1982; den Blanken and Hoff, 1982) it was shown that the sensitivity of ADMR was several orders higher than that of FDMR on the same material. This high sensitivity opened the way to ADMR studies of numerous

isolated RCs, pigment solutions, etc., both of bacterial and plant origin (reviewed in Hoff, 1989, 1990, 1993, 1996). Here, one example is given that highlights the power of especially LD-ADMR, which as explained above is similar to photoselection (in which an oriented distribution of e.g. photo-oxidized primary donors is produced by exciting the immobilized unoriented sample with a beam of linearly-polarized light). LD-(T - S) spectroscopy has the advantage that, in contrast to photoselection, the dichroic spectrum can be recorded with respect to two axes of reference that are perpendicular to each other. This reduces considerably the ambiguity of unraveling the orientation of the various transition moments in the T - S spectrum. Complex T - S spectra such as those of photosynthetic RCs, with many overlapping features such as appearing bands, bleachings, band shifts to the red and to the blue, can only be interpreted with any certainty if the corresponding LD-(T - S) spectra are available (Hoff et al., 1985).

The experimental T - S and LD-(T - S) spectra can be compared with spectra simulated with exciton theory, which describes the interaction between pigment molecules brought about by the electrostatic dipole-dipole coupling between their electronic transition moments. For two identical molecules this interaction causes a shift and a splitting of the excited state, which is now composed of two levels with (apart from the shift) energies given by the original energy plus or minus the interaction energy. The theory is easily extended to n pigments, each pigment interacting differently with the other $n - 1$ pigments (Davidov, 1981). For a known pigment configuration the absorption spectrum of the excitonically coupled spectrum is then readily obtained. Generally the resulting bands are mixtures of the original uncoupled bands, with transition moments that are vectorial combinations of the original transition moments. Thus, introducing a triplet state in a coupled pigment system, with corresponding changes in the dipole-dipole couplings, will in general lead to changes in the position, intensity *and* the polarization of individual absorption bands. Especially the change in polarization is useful for drawing conclusions on the extent of dipolar coupling between the optical transition moments of the cofactors in photosynthetic RCs.

The LD-(T - S) spectrum of RCs of *Rps. viridis* is

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displayed in Fig. 5. Exciton calculations based on the crystal structure of the RC of *Rps. viridis* (Deisenhofer et al., 1985) yielded a satisfactory simulation, when it was assumed that the triplet state is localized on the monomeric BChl component of D in the active chain (Fig. 5, drawn line), but not for localization on the BChl monomer in the inactive chain (Fig. 5, dashed line), or for a triplet delocalized on both BChls of the dimer (not shown).

In the past decade FDMR and especially ADMR and LD-ADMR spectroscopy have found wide application in the study of photosynthetic RCs and antenna preparations. Key results are the finding that isolated RCs generally exhibit a heterogeneity of the optical and magnetic resonance parameters of the primary donor, which is attributed to somewhat different conformations of the RC pigments, and the determination of the orientation of several transition moments. Both results are of crucial importance in the interpretation of the results of ultrafast pump-probe laser flash spectroscopy, and therefore for our understanding of the details of primary electron transfer.

Future applications of ODMR in photosynthesis will focus on comparative studies of mutant and chemically-modified RCs, and on RC heterogeneity. Pulsed ADMR will become increasingly important, allowing studies of the temperature dependence of the various triplet parameters, and of dynamical aspects of line-broadening, triplet-triplet transfer, etc. Recent results on the orientation of the various absorption bands in the T - S absorbance difference spectrum call for renewed effort in theoretically interpreting the optical properties of the RC pigment complex (Vrieze et al., *Biochim. Biophys. Acta*, in press).

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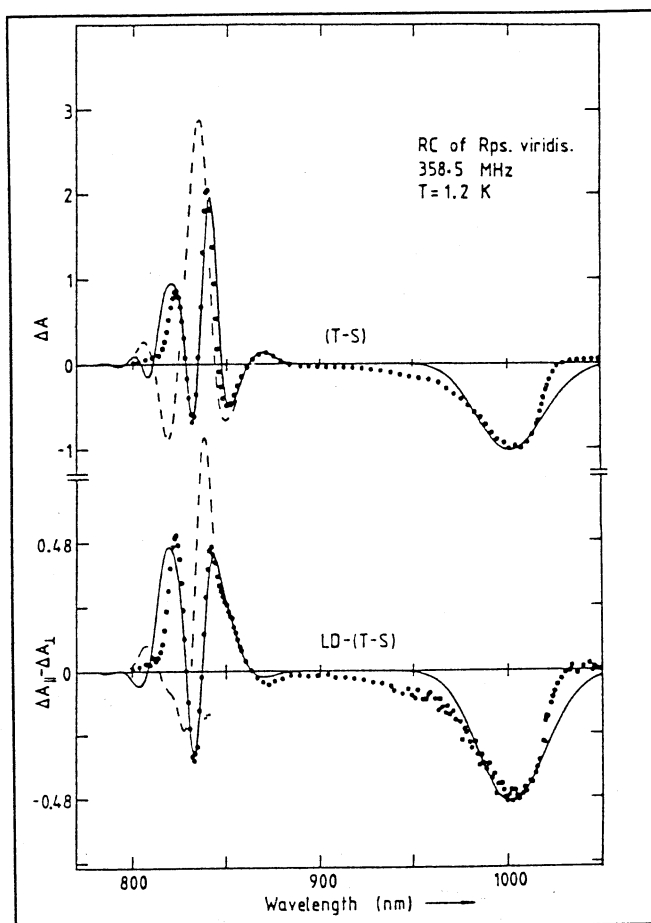


Figure 5: T - S spectra and LD-(T - S) spectra at 1.2 K of RCs of *Rps. viridis* for the ADMR transition at $|D| - |E|$. Dots: measured spectra. Drawn line: simulations assuming the triplet state of D localized on the D_A monomer. Dashed line: simulations assuming 3D to be localized on D_B . From Lous and Hoff (1987).

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Building The Perfect Beast

Chris Bender

NIH Biotechnology Resource for Pulsed EPR

MODIFICATION OF THE MIMS PROBEHEAD TO EXCLUDE LIQUID HELIUM

The Mims transmission resonator is a low Q structure that is well suited to pulsed electron spin resonance experiments. The body of the device is a brass block that is bolted onto a flange through which two parallel rectangular waveguides open (Figure 1). The probehead is typically used with a liquid helium immersion Dewar and therefore constructed in three sections (Figure 2): 1) a lower copper waveguide section that features coupling tapers; 2) a stainless steel heat barrier section; and 3) a copper waveguide bulkhead feedthrough. The joints are staggered and bolted together using half flanges (Figure 3).

For experiments requiring long term data acquisition, the Mims cavity suffers from a flaw in that the waveguide sections are porous to liquid helium, and the waveguide is therefore loaded with a fluid dielectric whose level changes with time. In other words, you will observe a phase shift as the helium level drops, and this is registered as a non-

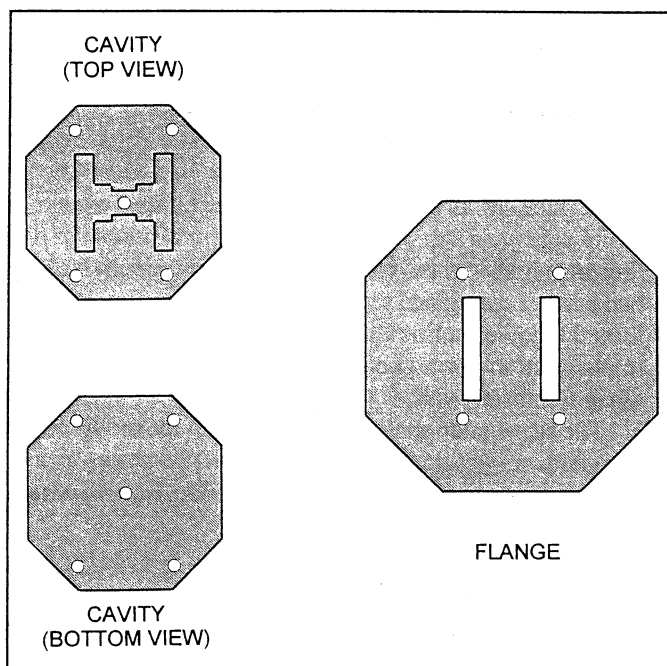


Figure 1: The Mims transmission resonator. The $\lambda/2$ strip and sample well are not shown.

exponential decay of the echo amplitude, which can affect the quality of the Fourier transform spectra. A HYSORE experiment without periodic tweaking of the reference arm phase would not be possible.

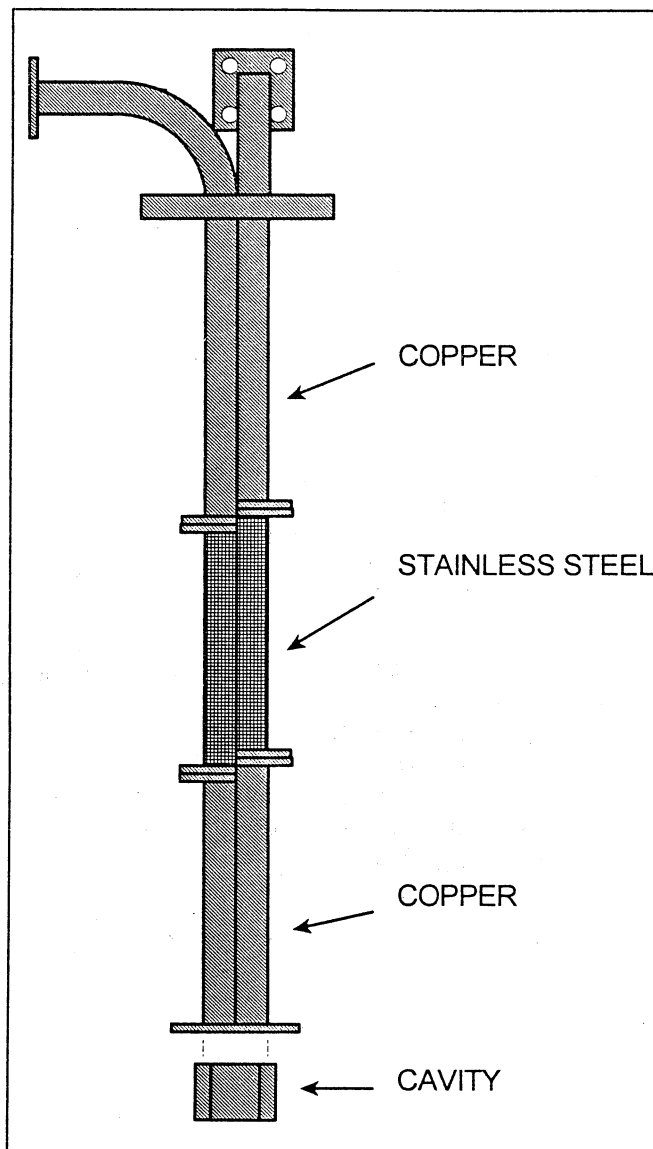


Figure 2: The Mims resonator probehead consisting of a parallel pairing of two waveguide transmission lines. A 12" stainless steel section serves as a heat barrier.

The brass block of the Mims 'cavity' is sufficiently heavy to keep a sample frozen once cooled to liquid nitrogen temperatures, and I ordinarily mount the probe onto the Dewar and run a few alternating cycles of vacuum/helium gas to displace all the atmospheric gas (with water vapor) from the waveguide. (The ports at the top of the Dewar have waveguide pressure windows.) This suffices to put a helium atmosphere in the waveguide prior to the liquid fill; it serves to prevent the condensation of gas on the interior of the waveguide and is truly useful only on days of high humidity. I find that displacing the ambient air in the Dewar/waveguide assembly with helium is most beneficial with probes that feature some mechanical part that must move freely (e.g. a Gordon coupler).

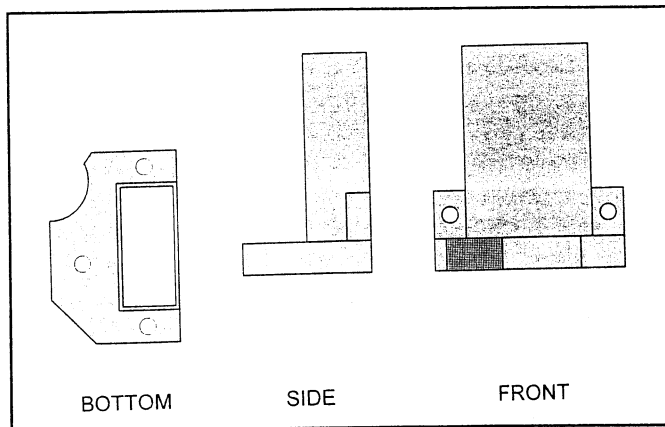


Figure 3: Half flange assembly for coupling adjacent waveguide sections.

One ordinarily uses a malleable metal such as indium to make vacuum seals in cryogenic systems, but the half-flanges that are used to prevent cross-talk between the transmitter and receiver waveguide sections are not conducive to a good indium seal because one runs out of flange on one side of the guide. There is a way to get a seal, however, if one makes a small modification to the waveguide wall and is careful during assembly.

The first step is to mill a hemisphere trench in the half flange (Figure 4). This will allow you to make a seal on three sides at the waveguide joint. In order to get a seal on the fourth side, mill a shallow trench in the wall of the guide against which the joint will butt. The trench is only used as a register to hold the indium ring against the joint; the posts

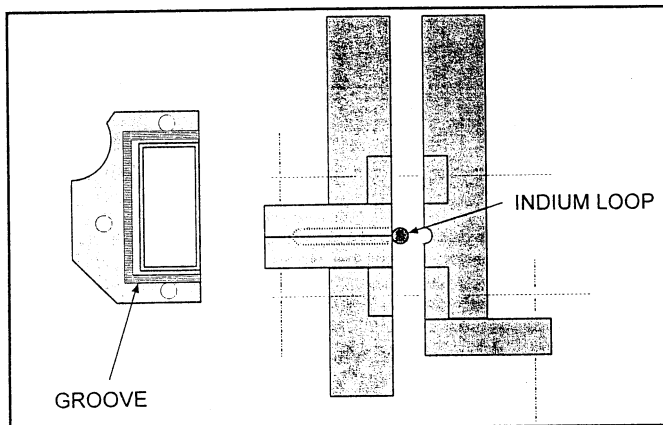


Figure 4: Placement of the groove for the indium wire on the half-flange. A loop extends to the outside of the waveguide and rests across the exposed joint. A groove in the adjoining waveguide wall holds the indium loop in place and horizontal clamps (screw positions indicated by dashed lines) compress the loop against the joint to make the seal. Not drawn to scale.

that are otherwise used to clamp the two parallel waveguide sections together in this case provide the pressure to compress the indium wire that seals the joint. Bear in mind that, since stainless waveguide is thinner than standard copper (0.020 vs. 0.050" walls), one needs to shim the stainless guide and use care with the solder joint at this position.

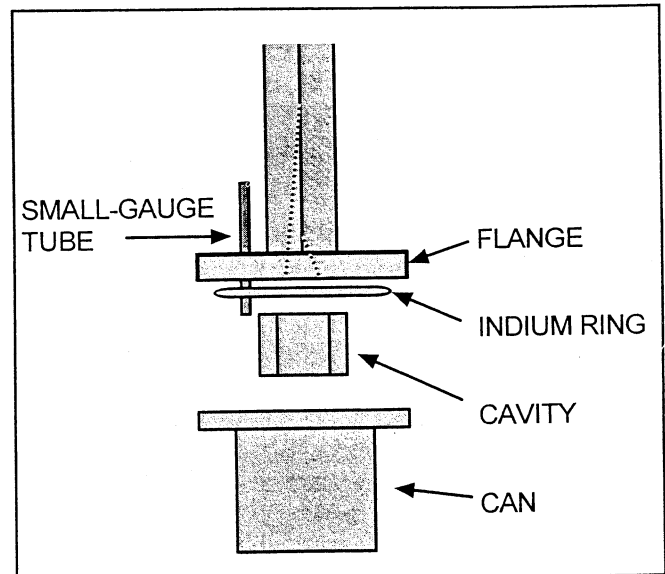


Figure 5: Detail of the cavity mount for a variable temperature Mims cavity. The can is sealed via an indium ring (cavity is not). Helium is drawn through the stainless capillary and exhausts through the waveguide section. Heater wires and temperature probes are not shown, and the stainless tube is not drawn in its entirety.

What often seems like the easier solution, namely brazing the steel and stainless sections together in a vacuum-tight butt (nested, or sleeve joint), turns out to be impractical. One first of all needs to use care in milling out the receptacle in the wall of the copper guide in order to get a flush fit, and then one has to worry about solder (and flux) residue within the guide. (Bill Mims once cautioned me about soft solder and superconductivity at helium temperatures.) On a fully assembled unit, it is also impossible to do a good job of soldering the joint on the inner face (the one where the two guide sections lies together). The flange that mates the cavity must span two waveguides and have a smooth surface (because it covers the cavity); although one could build the two parallel waveguide sections separately, they must still be joined together at this flange, and mere mortals will find it impossible to get a good solder joint (much less a braze) along the inside wall.

The waveguide sections outfitted with the modified seal are vacuum tight down to the flange that serves as a cavity

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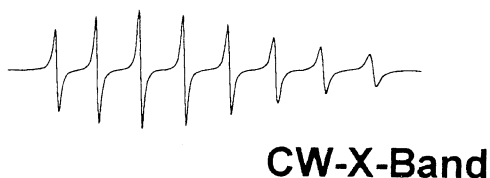
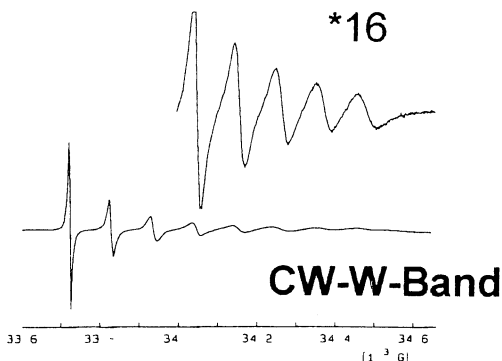
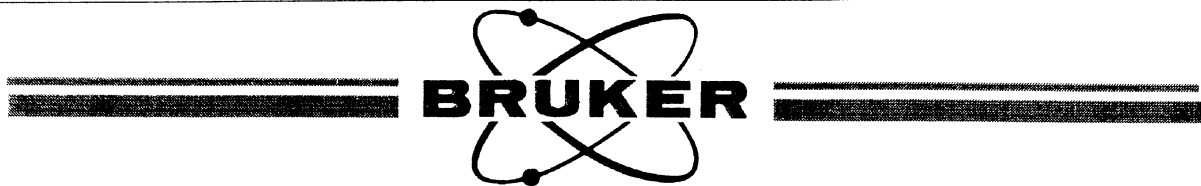
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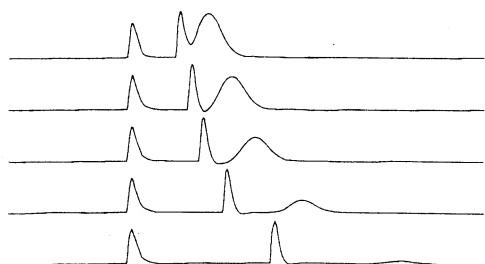
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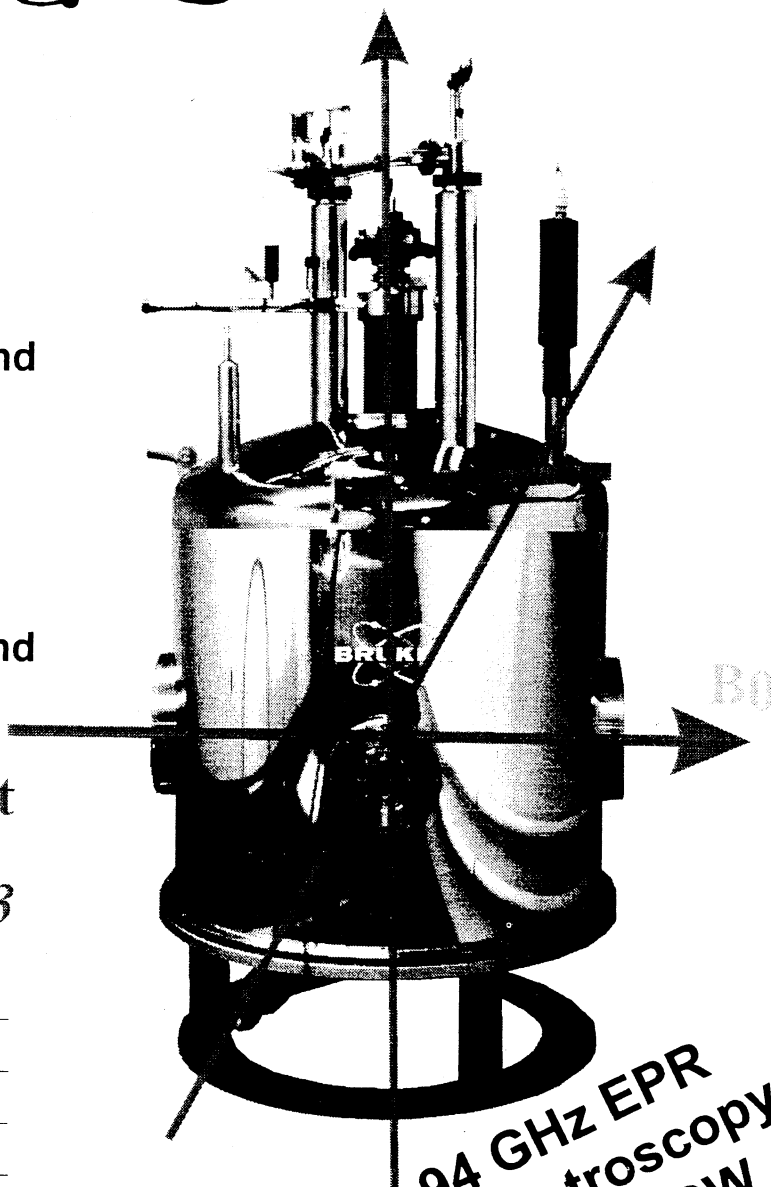


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mount. One can easily put an indium seal between this flange and cavity in order to seal the entire probehead, but I did not do this for two reasons: 1) the high voltage connection for LEFE is made through the cavity floor and will leak helium; 2) if I leave the cavity flange unsealed, I can make a variable temperature cavity. By putting a small vacuum port on a section of waveguide on the bulkhead outside the Dewar, a sealed can surrounding the cavity, and a narrow gauge tube that vents cold helium gas into the cavity chamber (Figure 5), I can use flowing helium gas as a heat exchanger.

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FABRICATION OF STAINLESS DOUBLE-RIDGED WAVEGUIDE

Part two of this issue's column addresses the problem of cryostat engineering. As described above, a 12" section of waveguide is used as a thermal barrier between the liquid helium and room temperature bulkhead; the waveguide has a very narrow wall (0.020 - 0.030"), and combined with the low thermal conductivity of the 304 grade stainless, the thin wall offers very little in the way of a heat conduit.

Stainless steel rectangular waveguide and tubing is commercially available (two suppliers listed below), and my X-, H-, and K_u-band probe heads feature standard WR-90, WR-75, and WR-62 stainless steel sections. We have wanted to extend our operating range downwards to C-band, however, and because the Mims cavity is geometrically scaled to the standard rectangular guide that feeds it, I was faced with the prospect of a very large cavity that would not fit within our helium immersion Dewar. (The dimension of WR-137 rectangular guide is 0.75 x 1.50", and therefore the parallel lines alone would be 3" square in cross-section, and about 4.25" across the diagonal.)

I was able to recover the compact size for a low frequency Mims cavity by switching to double (or single) ridged waveguide, which has a much smaller cross-section. The cavity, tapers, and bulkhead feed-throughs were no more difficult to make than the rectangular guide counterpart, but I was unable to find double ridged stainless guide. I was also frustrated in finding a shop that would do custom design work. I eventually settled on an electroformed nickel piece that is not as good a thermal barrier as stainless, but came as the only solution.

A while back I was rummaging in a used book store and picked up a book on jewelry making. I rationalize this kind of impulsive behavior by telling myself that I may learn some useful techniques for work (bribing administrators with homemade jewelry, for instance), and read about metal working methods.

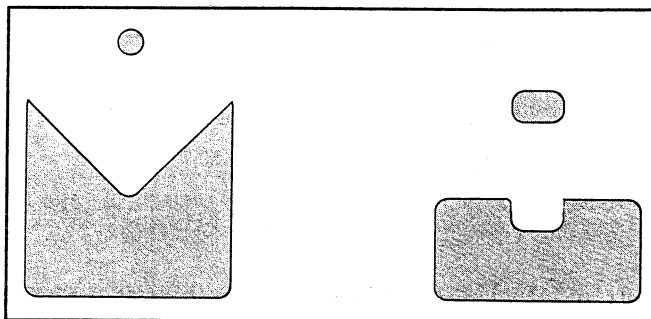


Figure 2-1

As it turns out, the jewelry making book had many useful chapters relevant to the manufacture of spectrometer components (Tiffany's jewelers is safe for now), one of them being sheet metal work. I can easily lay my hands on 304 stainless stock and persuade a welder (here's where all that

homemade jewelry comes in handy) to join finished parts, and so I decided to spend a couple of snowy weekends mangling metal.

I use two forms in metal fabrication. The first is a V-shaped form with a matching diameter rod. This form allows me to get a start on the bend for fitting into a tool die. I had a second tool die made by milling a 12" stainless bar (that is eventually tempered and hardened). The dimensions of the die match the interior of the stainless guide, and I specify rounded edges to prevent damage to the sheet as it is formed. A second narrow bar fits the slot (allowing for the thickness of the sheet stock). These parts are illustrated in Figure 2-1. The only other tool one needs is a soft faced hammer that will not mar the metal surface.

The procedure is illustrated in Figure 2-2. I hammer the

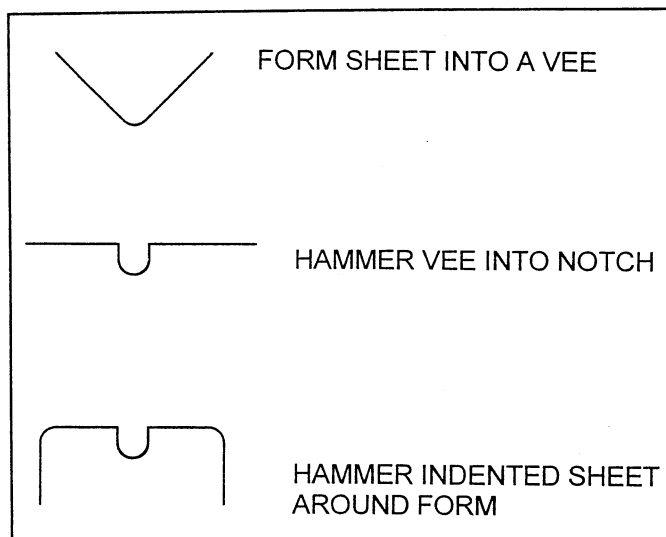


Figure 2-2

metal sheet stock into a rounded vee, then center the apex into the notch of the waveguide form. I position the narrow bar over the notch and pre-bent sheet and tap it snug into the notch. The sheet stock should take on the form of the ridge at this point, and I then proceed to form the metal around the remaining sides of the die.

If I want single ridged guide, I form the steel sheet completely around the tool die, and cut the sheet to size so that the seam lies along the narrow wall, which is then



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welded by a local shop. I get poor results if I try to wrap the sheet around on a double ridged form, however, and instead I hammer two sheets into a quasi-E shape. The two formed sheets are then cut to size and welded together, again along the narrow wall.

Lastly, a word about the metalworking. If you read the jewelry-making literature, you will find a lot written about shaping that entails the deformation of the metal (by deformation, I mean causing severe changes in thickness, density, etc.). It gives that 'artsy' handmade look (if you have ever seen Mauviel hammered copper cookware, you know what I mean). I am not using hammer blows hard enough to deform the metal in this work. For one thing, the steel sheet is springy, and the hammer is likely to bounce back in my face if I hit it too hard during the shaping around corners. But you will find that the steel responds fairly well to shaping without excessive violence.

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Penn Engineering Components, 12750 Raymer Street, North Hollywood, CA 91605, USA; ☎: (818) 782-2294 or (213) 873-3747.

OBSOLETE PARTS: Every now and then some component in an instrument fails and reduces me to a whimpering mass, particularly when I learn that the part is 'obsolete'. My traveling wave tube amplifier, for example, seems to have been (recently, I might add) totally constructed from obsolete

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parts. In a recent phone conversation with an engineer from Advanced Micro Devices, I apparently sounded so pathetic that he volunteered the name of two suppliers of obsolete parts (I had no idea that such places existed). For the benefit of others, they are:

(1) Rochester Electronics, 10 Malcolm Hoyt Dr., Newbury Port, MA 01950, USA; ☎: 508-442-9332. (2) Luke Systems: ☎: 818-991-9373 (USA) or 44-132928855 (UK).

TIPS & TECHNIQUES

Warning: Spin Labels Oxidize Common Buffer Substances under Radical Formation

Ralf M. Loesel, Anke Constantz, and
Wolfgang E. Trommer

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Good's zwitterionic buffer substances such as Tricine, Tes (Fig. 1), Hepes or Pipes have found wide biological applications. Although generally inert, the piperazine-derived buffers Hepes and Pipes (Grady et al., 1988) are known to form radicals by reaction with oxygen in the

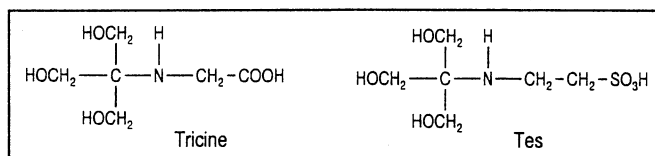


Figure 1: Chemical structure of Tricine and Tes.

presence of iron. In addition, Tricine radicals form upon oxidation with hydrogen peroxide (Grande and van der Ploeg, 1978). In the course of studies on chloroplast F_1 -ATPase with spin-labeled nucleotides (Vogel-Claude et al., 1988) in Tricine buffer we noticed a set of additional, rather narrow ESR signals at modulation amplitudes below 1 G (Fig. 2). In accordance with previous reports in the literature

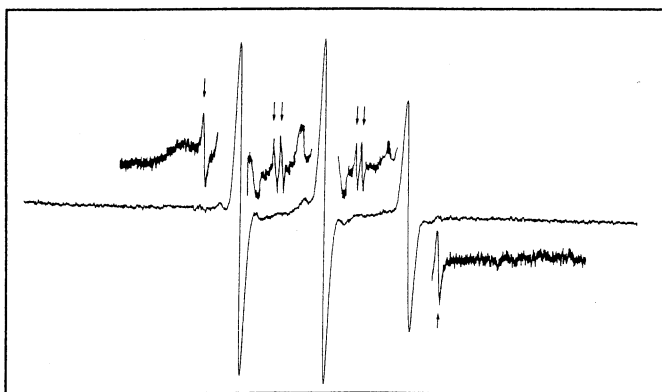


Figure 2: ESR spectrum obtained from CF1 ATPase with 2-N3-C2/3'-SL-ATP in Tricine buffer.

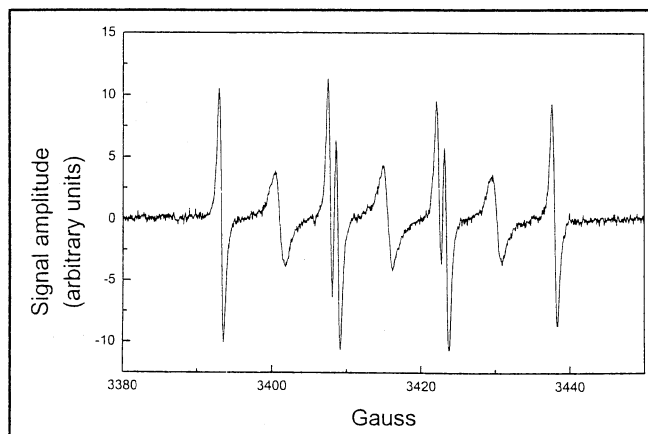


Figure 3: ESR spectrum obtained from 40 mM Tricine with 0.3 % hydrogen peroxide at pH 8.0.

(Grande et al., 1976, Graupe et al., 1989, Nett, 1992) we initially attributed these signals to additional hyperfine interaction with protons or even dipolar spin-spin-interaction between adjacent nitroxide radicals (Beth et al., 1984). However, we noticed that the additional signals are formed only in the presence of divalent cations as Mg^{2+} or Ca^{2+} and are readily lost with dithiothreitol (DTT). The reaction of hydrogen peroxide with Tricine generates a spectrum composed of narrow and broad lines (Fig. 3, first described by Grande and van der Ploeg, 1978), the former of which are superimposable with the unusual signals observed in our experiments. The same spectrum may be observed after irradiation of Tricine solution with flavin mononucleotide (FMN) in the presence of air.

The compounds formed from Tricine with nitroxide or hydrogen peroxide are likely to be identical, as the broader signals in Fig. 3 are probably buried underneath the residual signal of freely tumbling spin label in Fig. 2. This is corroborated by spectra recorded in the absence of enzyme (not shown).

The identity of the compounds was finally proven by separation of the radical formed from Tricine and Tempamine by ion exchange chromatography (DE 52, elution with water to remove Tempamine and subsequently, with 1M LiCl).

The buffer substance Tes is closely related to Tricine in its structure, differing only in a methylsulfonic acid moiety substituting for a carboxy function. With this compound, we did not observe Tempamine-dependent radical formation. However, hydrogen peroxide again generated a corresponding spectrum as shown in Fig. 4a. The spectrum and the corresponding stick diagram (Fig 4b) are easily explained in terms of two different methylene groups, presumably at the α -carbon atom ($a_H = 1.2$ G) and the β -carbon ($a_H = 0.9$ G), if no rotational restriction applies.

Hence, ESR studies with Good's buffers in the presence of potential oxidizing agents including nitroxide radicals may be severely hampered by artifacts due to buffer-derived radicals.

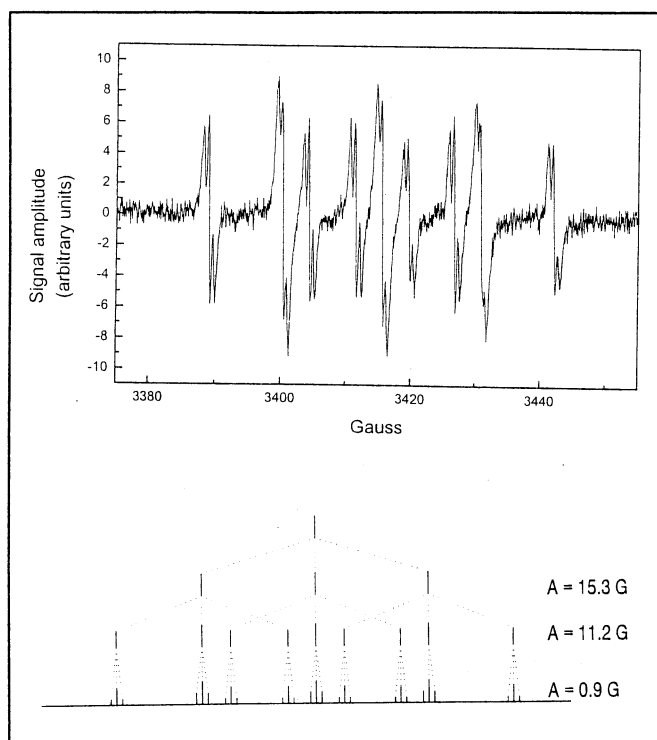


Figure 4: (a) ESR spectrum observed with Tes and hydrogen peroxide; (b) corresponding stick diagram.

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FROM EPR CENTERS

FROM the NATIONAL BIOMEDICAL CENTER for SPIN TRAPPING and FREE RADICALS, Oklahoma City, Oklahoma, USA:

At the last Spin Trapping Symposium (4ISST) in Oklahoma City in October, 1993, it was decided that the next conference should be held at York University, hosted by Dr. Michael Davies. The tentative date was set for March, 1996. However, in the meantime Dr. Davies has accepted a position in Australia; his new address is: The Heart Research Institute, 145-7 Missenden Rd., Camperdown, Sydney NSW 2050, Australia; ☎: 61-2-550-3560; FAX: 61-2-550-3302.

Further negotiations resulted in an invitation from the ESR Discussion Group which meets annually at various places in the UK with the primary discussion focus centered

on Organic/Biochemistry or Physical/Inorganic on alternate years. The former topic is scheduled for Spring 1997.

Thus, tentatively at this time, we have Prof. C.J. Rhodes hosting the ESR Discussion Group at Liverpool John Moores University towards the end of March, 1997. Professor Rhodes suggests that two days out of the meeting will be fully devoted to Spin Trapping topics. He has asked Dr. Ronald P. Mason and Dr. Edward G. Janzen, among others, to help organize this part of the meeting of the ESR Discussion Group. For further information, please write to: Prof. C.J. Rhodes, School of Pharmacy and Chemistry, Liverpool John Moores University, Byrom St., Liverpool L3 3AF, UK.

For more information, contact Dr. Edward G. Janzen, National Biomedical Center for Spin Trapping and Free Radicals, Oklahoma Medical Research Foundation, 825 NE 13th, Oklahoma City, OK 763104, USA; e-mail: edward-janzen@omrf.uokhsc.edu; FAX: 1-405-271-3980.

FROM the ILLINOIS EPR RESEARCH CENTER (IERC), Urbana, Illinois, USA:

The IERC can entertain proposals for collaborative research or for some service work, and we invite anyone interested to submit a short (a page or so) description of the problem and likely facilities needs. Preliminary contact with one of the IERC staff (e-mail ierc@uiuc.edu) is usually desirable. Techniques and instrumentation available at this Center include multi-frequency EPR (1 to 94 GHz), ENDOR, S-band ESEEM, and DNP relaxometry at 100 G. W-band (94 GHz) EPR can be used to resolve nearly-identical radicals, measure anisotropic motion down to the picosecond range, and provide very high point sensitivity for very small samples. A W-band station with liquid-helium cryostat and wide-field superconducting magnet sweep (0-7 T in ca. 15 min.) with separate high-precision fine sweep (up to 0.12 T range) is in operation. A remotely-controlled W-band sample goniometer for single-crystal rotation studies, developed in collaboration with Prof. John A. Weil (Univ. of Saskatchewan), can operate in the cryostat. For more information about facilities, personnel, and how to use the Center, visit the IERC web page: <http://ierc.scs.uiuc.edu>

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All of our units feature computer control and autotuning of the cavity and bridge. Our current magnet systems range from 4 to 12 inches. We have produced CW bridges for both X- and Q-bands. In addition, we have been involved in the repair and modification of existing systems and

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accessories. These modifications have included repair and replacement of bridges, field controllers, cavities, and temperature controllers. If you would like additional information on any of our systems, components, or assistance in the modification or repair of an existing system, contact us at: Summit Technology, Inc., 8827 Osceola Ave., Morton Grove, IL, 60053, USA, ☎: 1-800-735-6327 or 1-847-470-1638; FAX: 1-847-470-1562; e-mail: 73173.1415@compuserve.com; <http://ourworld.compuserve.com/hompages.summit1>.

COMMUNICATIONS & POWER INDUSTRIES

CPI Inc., formerly a division of Varian Associates, was formed in August 1995, and was made up of the Varian Electron Devices Group, Eimac Inc., and our Canadian Division. This company, Communications & Power Industries, will continue the same business focus using the same management (partial owners), people and locations, and will supply the same quality products as in the past.

Commercial markets such as klystrons are highly desired in today's business outlooks. Production of EPR klystrons is increasing and X-band klystrons will be available from stock soon. Q-band will become available as well, along with E-3 klystrons. This will allow our klystrons to fit all Varian E-line EPR spectrometers as well as Bruker klystron style spectrometers. These are direct replacements with liberal shelf life warranty and operating warranty. These replacements could easily extend the service life of the spectrometers another 10-20 years.

Our klystrons are tested on a Varian EPR spectrometer, using weak pitch as our standard, before delivery to insure quality for this demanding application. Life tests on this product line for X-band yield life times in excess of 50,000 hours which is supported by the long service life in the field of over 25 years in some cases.

CPI's contact person for EPR klystrons worldwide is James Anderson, Research Specialties, 5629 N. Maplewood, Chicago, IL, 60659, USA; ☎/FAX: 1-312-728-6570, or contact CPI Inc., formerly a division of Varian Associates, ATTN: Ed Niemann, 811 Hansen Way, Palo Alto, CA, 94304-1031, USA; ☎: 1-415-846-3188, FAX: 1-415-843-8780; ☎ toll-free: 1-800-843-8780.

NOTICES OF MEETINGS

THE FOURTEENTH INTERNATIONAL CONFERENCE ON RADICAL IONS, Uppsala, Sweden, July 1-5, 1996.

The Radical Ions conference is a continuation of previous Gordon Conferences 1968-1992 (totally 12) and the corresponding conference held in Halifax in 1994. Following our traditions, the conference will feature invited speakers and poster sessions with time for informal discussions. There will also be space for a number of short oral presentations.

The meeting will take place in the main building of Uppsala University, built in the center of Uppsala in the end of the last century. Uppsala is centrally located in Sweden, with excellent connections both by air (Arlanda airport), by train and by car.

The invited and contributed papers will be published in *Acta Chemica Scandinavica* as Minireviews, Articles or Short Communications, whichever is appropriate, and will be collected into a bound Symposium volume by the organizers. Regular refereeing procedures will be applied.

A significant part of the studies to be presented will involve EPR as a tool. Topics to be covered in the invited talks include:

- Spectroscopy and matrix isolation techniques.
- Radical ions in photochemistry and radiation chemistry
- Synthetic applications of radical ions
- Radical ions on surfaces
- Radical ions in biological systems
- Radical ions in electrochemistry
- Quantum chemical techniques

The registration fee is US\$250 for active participants. The cost for a first class hotel, centrally located, is approximately US\$70/night, breakfast buffet included, but there are cheaper accommodations in student dormitories that can be arranged. The total number of participants is limited to about 100. Acceptance will be on a first-come, first-served basis.

More details are available in a first circular that will be distributed to those interested in attending the conference. To obtain the circular, contact Mari Lofkvist, Secretary, RADICAL IONS 14, Department of Physics, IFM, Linköping University, S-581 83, Linköping, Sweden. For further information about the scientific programme please contact one of the chairmen: Anders Lund, Dept. Physics, IFM, Chemical Physics Laboratory, Linköping Univ., S-581 83, Linköping, Sweden, FAX: 46-13-13-22-85, E-mail: ald@irm.liu.se; Sten Lunell, Dept. Quantum Chemistry, Box 518, Uppsala Univ., S-751 20, Uppsala, Sweden. Or communicate by FAX or E-mail: FAX: 46-18-50-24-02, E-MAIL: lunell@kvac.uu.se.

EPR AND d-TRANSITION METAL CHEMISTRY, Univ. Manchester, UK, July 5, 1996.

The Symposium *EPR and d-Transition Metal Chemistry* celebrates the opening of the EPSRC Service centre for CW EPR spectroscopy and Frank Mabbs' contributions to chemistry following the occasion of his 60th birthday (August 1995). It is sponsored by The Royal Society of Chemistry Dalton Division; Bruker Spectrospin and British Nuclear Fuels Limited. Speakers will include: Prof. C.D. Garner (Univ. Manchester, UK), Prof. M. Schröder (Univ. Nottingham, UK), Prof. N.M. Atherton (Univ. Sheffield, UK), Prof. J.H. Enemark (Univ. Arizona, USA) and Prof. The Lord Lewis (Univ. Cambridge, UK). Registration is £5 (please make cheques payable to the Univ. of Manchester). For more information, contact Mrs. Y.K. Cope, University of Manchester, Dept. of Chemistry, Manchester M13 9PL, UK; ☎: 44-161-275-4653; FAX: 44-161-275-4616; e-mail: dave.garner@man.ac.uk.

NINETEENTH INTERNATIONAL EPR SYMPOSIUM at the 38th Annual Rocky Mountain Conference, Denver, CO, USA, July 21-25, 1996.

This conference has become a traditional major annual event. At this year's symposium, Prof. Kev Salikhov (Zavoisky Institute, Kazan) will present his award address for the Gold Medal of the International EPR (ESR) Society (IES). Prof. Klaus Möbius (Freie Universität, Berlin) and Dr. Ronald Mason (National Institute of Environmental Health Sciences) will present award addresses for the Silver Awards of the IES, and Dr. Gunnar Jeschke (ETH Zürich, Lab. Physical Chemistry, Zürich, Switzerland) will present an IES Young Investigator Award address.

Ron Mason has organized a special session on nitric oxide in medicine and biology (Tuesday, July 23), and there will be an instrumentation session (Thursday, July 25).

Extensive information on this conference, including details on program and events, may be found on the World Wide Web site. The URL is

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

Or contact: Prof. Sandra S. Eaton, Univ. Denver, Dept. Chemistry, Rm. 153 Seely G. Mudd Science Bldg., Denver, CO 80208, USA; ☎: 1-303-871-3102; FAX: 1-303-871-2254; E-mail: seaton@du.edu or Prof. Gareth R. Eaton, Univ. Denver, Dept. Chemistry, Denver, CO 80208, USA; ☎: 1-303-871-2980; FAX: 1-303-871-2254; E-mail: geaton@du.edu.

XVIIth INTERNATIONAL CONFERENCE ON MAGNETIC RESONANCE IN BIOLOGICAL SYSTEMS, Keystone, Colorado, USA, August 18-23, 1996.

This is the first meeting in this biennial series to be held in North America since 1988.

Conference Program. A broadly based program has been planned, covering new magnetic resonance methods, applications of high resolution NMR to structural biology,

application of solid state NMR techniques, use of EPR in studying a variety of paramagnetic systems, *in vivo* spectroscopy and imaging, and a minisymposium on Biomolecular NMR and Drug Discovery. The conference will feature 12 plenary lectures, along with about 80 invited lectures and 25 short talks in three parallel sessions. Three poster sessions, each accommodating up to 200 posters, will permit participation by a large number of workers active in many aspects of biological magnetic resonance.

Conference locale. The meeting will be held at the Keystone Conference Center, which has been the site of several conferences on protein NMR. Keystone is a planned resort community in the Rocky Mountains, about 75 miles west of Denver. Most air travelers will fly to the new Denver International Airport, which has good domestic and international connections. Rental cars and shuttle buses are available from the Denver Airport to Keystone. The Conference Center, opened in 1989, will be the site of all lecture and poster sessions, with coffee breaks and display of vendor materials in the foyers and terraces. The nearby Keystone Lodge will provide space for commercial exhibitors and hospitality suites. The Keystone Resort includes two hotels, with 255 rooms, as well as 800 condominium units. There are many restaurants in all price ranges and full recreational facilities for swimming, boating, golf, tennis, hiking and trail riding. During August the weather at Keystone is usually very pleasant, with daytime high temperatures running 20° to 30°C.

For further information, contact the Conference Office, attn: Judith A. Sjöberg, Conference Manager, at 1201 Don Diego Ave., Santa Fe, NM 87505 USA; ☎: 1-505-989-4735; FAX: 1-505-989-1073. A page has been established on the World Wide Web; the URL is:

<http://nmrsgil.ncifcrf.gov/icmrbsxvii>

This Web site aims to provide updated information on the conference program as it is developed.

28th CONGRESS AMPÈRE on MAGNETIC RESONANCE, University of Kent, Canterbury, UK, September 1-6, 1996.

The meeting will be held at the University of Kent, located on a hillside overlooking Canterbury. The ancient city of Canterbury is famous throughout the world for its magnificent Cathedral. This beautiful building has played an important role in history and it contains the tombs of royalty, archbishops and cardinals. All accommodation and meals will be on the University Campus. The University of Kent is well served by road and rail from the major London airports, the south coast ports of Dover and Ramsgate and the Channel Tunnel. Given sufficient demand, arrangements will be made for coach travel to and from Heathrow and Gatwick airports.

A series of parallel sessions will be held on a wide variety of magnetic resonance topics. These will consist of invited and contributed oral presentations and two poster sessions. Topics include:

- EPR, NMR, NQR and μ SR
- Diffusion and molecular motion
- Disordered and advanced materials
- Microimaging
- Modern developments in solid state NMR
- Multi-dimensional, quantum and resonance spectroscopy
- New Methods and approaches
- Non-equilibrium and non-linear phenomena
- Liquid crystals
- Polymeric materials
- Superconductors, diamonds
- Spin dynamics

A conference excursion, banquet and entertainment will be available together with a social program for accompanying guests.

In view of the commemorative nature of the meeting to celebrate some important historical magnetic resonance events, a key feature will be short plenary lectures from B. Bleaney (Oxford), R.V. Pound (Harvard), Y. Servant (Bordeaux) and J.G. Powles (Kent).

Invited speakers include: J.P. Amoureux (Lille), M. Armand (Grenoble), P.T. Callaghan (Massey), P. Carretta (Pavia), S.J.F. Cox (RAL), H. Eckert (Münster), J. Emsley (Southampton), D. Goldfarb (Wieżmann), W.P. Halperin (Northwestern), J. Miller (Naval Research), K.A. Muller (IBM), M. Newton (Oxford), P. Reidi (St. Andrews), K. Salikhov (Kazan), A. Samoilenko (Moscow), J. Schmidt (Leiden), J.M. Spaeth (Paderborn), J. Titman (Nottingham), R. Tycko (Bell Labs), C. Yannoni (IBM), D.B. Zax (Cornell).

The organising committee consists of Prof. J.H. Strange (Chairman), Dr. M.R. Halse (Secretary), Dr. M.E. Smith (Secretary), Dr. E.R.H. van Eck, Dr. P.C.L. Stephenson, Dr. P.J. MacDonald (Surrey), Dr. J.M. Baker (Oxford), Prof. Sir P. Mansfield (Nottingham), Prof. P. Morris (Nottingham) and Prof. E.F.W. Randall (Queen Mary, London).

All prospective participants are asked to register by May 15, 1996. More detailed information can be obtained by contacting The Secretariat, 28th Congress Ampère, The Physics Laboratory, University of Canterbury, Kent CT2 7NR, UK; ☎: 44-0-1227-823767; FAX: 44-0-1227-827558; e-mail: AMPÈRE@ukc.ac.uk.7

ELECTRON PARAMAGNETIC RESONANCE of RADICALS and METAL COMPLEXES, 2nd International Conference of the Polish EPR Association, Warsaw, Poland, September 9-13, 1996.

General Information: The 2nd International Conference will be held in Warsaw in the Parkowa Hotel (accommodations and conference center) and Uniwersytecki Hotel (accommodations) both on Belwederska Street, near Lazienki Park.

Scope & Topic of the Conference: A broad range of problems which can be solved or helped by the use of EPR spectroscopy; its application in such fields as chemistry, biochemistry; physics and bio-physics; studies on paramagnetic

intermediates generated by radiolysis and photolysis; technical aspects and modern trends in EPR spectroscopy and related techniques.

The following scientists have so far agreed to present plenary lectures (or to attend the conference): A. Alberti (Italy), D. Beckert (Germany), M. Brustolon (Italy), F. Callens (Belgium), A.G. Davies (UK), F. Gerson (Switzerland), B.C. Gilbert (UK), D. Goldfarb (Israel), A. Jezierski (Poland), L. Kevan (USA), H. Kurreck (Germany), Ya.S. Lebedev (Russia), A. Lund (Sweden), K.A. McLauchlan (UK), A. Plonka (Poland), E. Reijerse (Netherlands), S. Schlick (USA), M.D. Sevilla (USA), J. Stankowski (Poland), M.C.R. Symons (UK).

The social program will include an excursion, a conference dinner, an opera performance or concert, and sightseeing around Warsaw's Old City.

The Organizing Committee consists of Prof. Andrzej Chmielewski, Assoc. Prof. Hanna B. Ambroź, Assoc. Prof. Jacek Michalik, Dr. Zbigniew Zimek (all of the Institute of Nuclear Chemistry and Technology) and Prof. Zbigniew Kęcki (University of Warsaw).

For further information please contact Assoc. Prof. Hanna B. Ambroź, Inst. Nuclear Chemistry & Technology, ul. Dorodna 16, 03-195 Warsaw, Poland. ☎: 48-22-11-23-47, FAX: 48-22-11-15-32.

FIRST INTERNATIONAL SEMINAR ON SIMULATION MODELING IN BIOENGINEERING (BIOSim 96), Merida, Venezuela, October 24-25, 1996.

The objective of this International Seminar is to bring together scientists who are carrying out research on the applications of computers to simulate biomedical problems. The Conference will be held at the Cultural Centre 'Tulio Febres Cordero', Merida. Conference topics will include:

- *Simulation of Physiological Processes*
- *Biomedicine*
- *Electrical and Magnetic Simulation*
- *Imaging Processing*
- *Data Acquisition and Analysis*

Inquiries about the Seminar should be sent as soon as possible to Sue Owen, Conference Secretariat, BIOSim 96, Wessex Inst. Technology, Ashurst Lodge, Ashurst, Southampton, SO40 7AA, UK;

☎: 44-1703-293223; FAX: 44-1703-292853;

E-mail: cmi@uk.ac.rl.ib; Intl. E-mail: cmi@ib.rl.ac.uk.

FIFTH INTERNATIONAL WORKSHOP ON ELECTRON MAGNETIC RESONANCE OF DISORDERED SYSTEMS (EMARDIS) and 2nd INTERNATIONAL SEMINAR ON APPLIED EPR, June 1997, Sophia, Bulgaria.

The Fifth International Workshop on Electron Magnetic Resonance of Disordered Systems (EMARDIS) and the Second International Seminar on Applied EPR (APPL-EPR), which will be held in June 1997, near Sofia, will be

organized by Bulgarian EPR Society in collaboration with the Institute of Catalysis, Bulgarian Academy of Sciences and the Department of Chemistry, Sofia University. The official language for both meetings is English.

Scope. The aim of the EMARDIS workshop is to cover all qualitative (structure-reactivity relationships, kinetics, etc.) aspects of recent development in the theory, methodology, instrumentation, experiment, etc. of the Electron Magnetic Resonance (EMR = EPR, ENDOR, ESE) spectroscopy of disordered systems. The discussions on APPL-EPR will cover the Fundamental aspects of Quantitative EPR (theoretical and practical considerations of the Q-EPR, standards, calibration, metrology, methodology, instrumentation - new methods, advanced techniques, automation, etc.) as well as continuously extended applications of EPR in all fields of science, technique and practice (dosimetry, environmental and food preservation control, medicine, geology, archeology, petrol industry, polymer chemistry, etc.). The above topics will be covered by lectures, posters and round-table discussions. In order to ease scientific contacts and discussions on the individual level, the number of participants in each meeting will be limited to about 40 persons.

The EMARDIS workshop will begin with dinner on Monday and end on Friday after breakfast. The APPL-EPR Seminar will begin with a dinner on Friday and will close on Monday after breakfast. In this way, those who are interested in only one topic will have the opportunity to save time by attending the meeting of their choice.

Publications. As in previous EMARDIS and APPL-EPR meetings, there will be two different kinds of publications: short abstracts of all presentations available in both meetings, full length of the invited lectures, and a selection of short communications will be published in a special issue.

Social Programme. A welcome party, farewell dinner, and a half-day visit to Sofia are planned, free to all EMARDIS and APPL-EPR participants. In addition, Friday is planned to be an optional free/excursion day to some places of national and/or historical significance.

Further Information. A first circular of both meetings will be distributed in September 1996. The Organizers request recipients to kindly fill out and return the attached preliminary registration form as soon as possible, even those who do not plan to attend the workshop. This way, they will know that their mailings have not gone astray.

All correspondence should be addressed to: N.D. Yordanov (Convener), Institute of Catalysis, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria, fax: 3592-756-116 or 720-038; ☎: 3592-713-2546 or -3917; telex: 22729 ecbhan, e-mail: NDYEPR@BGEARN.ACAD.BG

THIRD EUROPEAN ESR MEETING, August 25-29, 1997, Leipzig, Germany.

The III European ESR Meeting will be held August 25-29, 1997 in Leipzig, Germany. The title is "Modern Aspects

of Structure and Dynamic Investigations of Paramagnetic Systems by EPR".

Topics will include:

1. Recent advances and applications of modern methodical developments
 - High field and high frequency ESR
 - Pulsed techniques and transient methods
 - Combination of ESR and optical methods
 - Electrical detected ESR
 - Computer supported ESR analysis
 - Imaging
2. New trends in physical applications
 - Local order and dynamics in solids, glasses and polymers
 - Defect structure and material properties
 - Characterization of Fullerenes
3. New trends in chemical applications
 - Reaction kinetics in fluid and solid systems
 - Spin polarization effects and magnetic field effects
 - Spin trap chemistry
4. New trends in biological applications
 - Metal ions in complexed bioinorganic systems
 - Photosynthesis
 - Radical damage of DNA and proteins
 - Oxidative stress in biological systems

For more information, contact DP Dr. Habil. Dieter Beckert, Max-Planck-Society, Research Unit "Time Resolved Spectroscopy" at the University Leipzig, Permoserstr. 15, D-04303 Leipzig, Germany; ☎: 49-341-235-2630; FAX: 49-341-235-2317; E-Mail: beckert@mpgag.uni-leipzig.de

POSITIONS AVAILABLE & WANTED

POSITIONS AVAILABLE

A Full-time position is available for an individual with expertise in programming (C and FORTRAN), EPR instrument repair, and general EPR spectroscopy to work with a biological ESR group. Although research opportunities will be available, the major responsibilities will be to support and educate post-doctoral researchers who are not trained as ESR spectroscopists. The position is with a Federal contract firm (U.S. citizen or permanent resident only). Please send *curriculum vitae* to Ronald P. Mason, NIEHS/NIH, P.O. Box 12233, Research Triangle Park, NC, 27709, USA.

Physicist/Chemist/Materials Scientist Postdoctoral Position in Electron Spin Resonance. The Center for Materials Research (CMR) at Norfolk State University (NSU) invites applications for an expected postdoctoral

research associate position with a June 1, 1996 starting date (negotiable). The successful candidate will be responsible for investigating inorganic crystals and/or polymeric materials using a new Bruker EMX X-band/Q-band electron spin resonance spectrometer with 1.3 T rotating base magnet and Oxford Scientific low temperature cryostat. The NSU CMR has major research collaborations with NASA Langley Research Center (in nearby Hampton, VA) and Los Alamos National Laboratory. There is a possibility that this position could be converted to tenure-track after two or three years. Candidates should submit a curriculum vita, a statement of research interest, and arrange for three letters of reference to be sent to: Dr. Heidi R. Ries, Associate Director, CMR, Norfolk State Univ., Norfolk, VA, 23504, USA; e-mail: h_ries@vger.nsu.edu. Screening of applicants will begin immediately and will continue until the position is filled. NSU is an Affirmative Action/Equal Opportunity Employer.

Illinois State University—Tenure track position at the Assistant Professor level to begin in January, 1997. Ph.D. required and postdoctoral experience desirable. Development of a productive research program involving B.S. and M.S. students that will attract external funding will be expected. Significant involvement and a strong commitment to teaching in the General Chemistry program is also expected in addition to teaching in area of specialization. To receive fullest consideration applicants should submit a resume, a brief description of proposed scholarly projects, and the names of at least three references to Chairperson, Department of Chemistry, Illinois State University, Normal, IL 61790-4160 before May 31, 1996. An Equal Opportunity/Affirmative Action Employer. Michael E. Kurz, Dept. Chemistry, Illinois State Univ., Normal, IL, 61790-4160, USA; ☎: 1-309-438-7661; FAX: 1-309-438-9257; e-mail: mkurz@rs6000.cmp.ilstu.edu.

POSITIONS WANTED

EPR spectroscopist seeks academic or industrial position. Physical chemist, now postdoctoral fellow in Chemistry Dept., Univ. Houston. Education: M.Sc. Molecular Spectroscopy, 1985, Warsaw Univ., Warsaw, Poland; Ph.D. ESR of silver clusters in zeolites, Inst. Nuclear Chemistry and Technology, Warsaw, Poland. Research experience: liquid and powder ESR in chemistry and radiation chemistry, ESR and ESEEM of paramagnetic transition-metal ions in zeolites and other microporous materials, synthesis of microporous materials, ESR dosimetry, ESR examination of irradiated foodstuffs. Experience in maintenance of Bruker ESR spectrometers (200, 300 and 380 series) and their additional equipment, computerized data-processing, ESR and ESEEM simulations. Looking for a research post or opportunity to teach basic principles of magnetic resonance spectroscopy.

Contact Dr. Tomasz Wasowicz, Chemistry Department,
University of Houston, Houston, TX 77204-5641, USA;
☎: 1-713-743-3251; FAX: 1-713-743-2709;
e-mail: wasowicz@jetson.uh.edu
or wasowicz@orange.ichtj.waw.pl.

EQUIPMENT & SUPPLIES EXCHANGE

KLYSTRONS AVAILABLE

Varian klystrons are now available from CPI Inc., formerly a division of Varian Associates. The Varian Microwave Power Tube Division was sold to CPI Inc. last August. CPI has the same people and facilities as before, plus the same international offices. As of March 1996, klystrons will be available from stock. Jim Anderson of Research Specialties is acting as CPI's contact person for EPR klystrons worldwide. Contact Jim Anderson, Research Specialties, 5629 N. Maplewood, Chicago, IL 60659, USA; ☎/FAX: 1-312-728-6580. Or, contact CPI Inc., formerly a division of Varian Associates, ATTN: Ed Niemann, 811 Hansen Way, Palo Alto, CA 94304-1031, USA; ☎: 1-415-846-3188, FAX: 1-415-843-8780.

FOR SALE: USED VARIAN SPECTROMETER

Used Varian E-4 X-band EPR spectrometer with E-231 cavity and an E-257 variable temperature accessory. Excellent condition with low hours of use. Will be sold as a reconditioned unit meeting original factory specifications with warranty. Call for details, James R. Anderson, Research Specialties, 5629 N. Maplewood, Chicago, IL, 60659, USA; ☎/FAX: 1-312-728-6570.

WANTED

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

WANTED: EPR CAVITY

The Institute of Mineralogy, University of Marburg, Germany is looking for an EPR cavity for a Varian Model E-110 EPR, Q-band spectrometer. We would like to acquire a used cavity. If you have one available please contact Stefan Hafner, Inst. Mineralogy, Univ. Marburg, 35032 Marburg, Germany; FAX: 49-6421-288919; E-mail: hafner@mail. uni-marburg.de.

JEOL TE2000 SPECTROMETER

JEOL has a TE2000 EPR spectrometer in stock in Boston that they are willing to let go at a substantial

discount. For further information, contact Robert DiPasquale at dipas@jeol.com.

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@du.edu; ☎: 1-303-871-2419.

FOR SALE: VARIAN SYSTEM

Micro-Now Instruments presently has available:

- 1) a VARIAN Century series console with field dial regulator, high and low frequency modulation units, Models E207 and E204, oscilloscope and digital drive recorder
- 2) a E110 Q-band Bridge with cavity
- 3) a Low-frequency modulation unit, module model 921507, E204
- 4) replacement Klystrons for Varian EPR Bridges (at reduced prices)
- 5) Model V4533 VARIAN EPR TE011 mode, rotating cylindrical cavity
- 6) VARIAN general purpose cavity E231

For more information on these units contact Clarence Arnow, President of Micronow:

Voice phone: 708-677-4700; FAX: 708-677-0394
E-mail: mninco@wwa.com.

ANNOUNCEMENTS

MAILING LISTS FOR SCIENTIFIC MEETINGS

If you are planning a scientific conference, you may contact an officer of the International EPR Society or the IERC (address on front page of this Newsletter) to obtain a list of the 1,300+ Society members for use in issuing invitations. If you would like to have preprinted mailing labels, Martha Moore, who provides secretarial support for the Society, can do this at cost -- approximately \$50.00 (includes cost of labels, postage and, if you wish, a disk copy of the list in ASCII format). Labels for the entire database (3,800+ members and non-members) would cost approximately \$175.00.

1996 MEMBERSHIP DUES

IES Members: Have you paid your dues? It's easy to lose track. If you are not sure, it will save the Society the expense of mailing dues notices if you will take a moment to ascertain the status of your membership according to our records. To do this, please check the lower right hand corner of your mailing label. You will find there four dashes ("-- --"). If only the four dashes "-- --" or "--0--" appear, no dues have been recorded for you for the 1996 year. If dues

have been paid, either a numeric value or the letter "R" or "C" (for soft currency countries) will appear, e.g. "--30--" or "--R--".

IES DUES PAYMENT RECORDS ON WWW

As of February 15, 1996 a list of all members whom the International EPR Society's records show as having paid dues in 1994, and/or 1995, and/or 1996 was placed on the World Wide Web, so members may check to see whether their dues payments have been reported and properly recorded in the IES files at the IERC. We plan to update the list the middle of each month, so do allow time for recent payments to be placed on the list. The WWW address is: <http://ierc.scs.uiuc.edu/IES.html/>. If you do not have convenient access to the web, or have a question, contact us at ierc@uiuc.edu. Please note that, owing to database limitations, all dues paid in hard currency are reported in US\$ and all dues paid in soft currency are shown as "C" or "R." If you have not paid dues for 1996, a form for dues payment is on this web site along with methods to pay dues, depending on where in the world you are located.

NIH FORMS AVAILABLE ON WEB

The newly-revised PHS 398 forms to apply for NIH research grants in the USA are available over the World Wide Web from Rice University. The web site is:

<http://tram.rice.edu/TRAM/>

Forms are available in both Microsoft Word and WordPerfect formats.

"APPLIED MAGNETIC RESONANCE" SPECIAL OFFER FOR IES MEMBERS

[Note from the editor: We have received from IES officers and Springer-Verlag publishers the following announcement renewing the offer to make the Journal that Prof. Kev Salikhov edits available to IES members at a tiny fraction of the usual price. I already am taking advantage of this generous arrangement; I am very pleased with it and urge other IES members to consider subscribing. R. Linn Belford]

Springer-Verlag offers you, as a member of the International EPR(ESR) Society, the journal *Applied Magnetic Resonance* at a vastly discounted personal rate. Instead of the annual non-member subscription price of US\$847, you pay only US\$92 plus US\$40 postage; i.e., you save US\$705 per year.

On these terms, can you afford NOT to subscribe today? *Applied Magnetic Resonance* provides an international forum for the application of magnetic resonance in physics, chemistry, biology, medicine, geochemistry, ecology, engineering, and related fields. The journal publishes original articles with a strong emphasis on new applications and new experimental methods. In addition, special issues are dedicated to specific fields of magnetic resonance.

Use this order form for **Applied Magnetic Resonance**:

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I affirm that I am a member in good standing of the International EPR (ESR) Society, and therefore claim my members-only discount price.

Signature: _____

Method of payment: Bill me Check enclosed

Charge my credit card:

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Card number: _____

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FUTURE POSSIBLE SOURCE OF TRAVEL FUNDS FOR WOMEN

Following the tragic death on October 31, 1995 of our beloved colleague, Dr. Maria Pia Gratton, physicist and systems analyst at the University of Illinois School of Chemical Sciences, Urbana, IL, a fellowship fund was established in her memory. The fund provides a \$5,000 stipend and a waiver of tuition and fees to allow a female student from another country to have an academic and cultural experience at the University of Illinois at Urbana-Champaign. Later this year, applications for 1997 will be accepted. To obtain more information concerning Pia and this fund, access the following World Wide Web site:

<http://www.scs.uiuc.edu/~skypen/pia/manifest.html>