Volume 8, Number 1

Page 1

Spring/Summer, 1996

- 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 these 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. 2: 414-456-4008. FAX: 414-266-8515.

E-Mail: cfelix@post.its.mcw.edu

WWW: http://www.biophysics.mcw.edu/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.

**2**: 718-430-2175. FAX: 718-430-8935.

E-mail: peisach@aecom.yu.edu WWW: http://spin.aecom.yu.edu

#### Illinois EPR Research Center (IERC),

Fram the Piliter

Prof. R. Linn Belford, Director; Prof. Robert B. Clarkson, CoDirector; Prof. Peter C. Debrunner, Assoc. Director, Prof. Mark J. Nilges, Asst.. Director, Dr. Alex I. Smirnov, Laboratory Manager; Asst.. to Directors, Ms. Becky Callivan.

University of Illinois at Urbana, 190 MSB, 506 South

Mathews, Urbana, IL, 61801, USA.

☎: 217-244-1186. FAX: 217-333-8868.

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

#### IN THIS ISSUE

ternational EPR(ESR) Society Affairs
From the President (K. McLauchlan) PR Specialist Vignettes (A. Schweiger, ed.) The Linear Electric Field Effect in EPR (W.B. Mims)
PR Specialist Vignettes (A. Schweiger, ed.)  The Linear Electric Field Effect in EPR (W.B. Mims)
The Linear Electric Field Effect in EPR (W.B. Mims)
(W.B. Mims) 2-4 Cuest Editorial (H.M. Swartz) Lessons for the EPR Community from the 1996
Guest Editorial (H.M. Swartz)  Lessons for the EPR Community from the 1996
Lessons for the EPR Community from the 1996
Primary Election Campaign in the USA 4-5
uilding the Perfect Beast (C. Bender)
rom EPR Centers9
otices of Meetings 9-12
ositions Available & Wanted
quipment & Supplies Exchange
nnouncements
(Weil Honored; Mailing lists; Info. on WWW;
E-mail updates)
ppendices: IES Directory, Directory on Research Fields 16-47

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

### From the Editor—

This is the annual Directory edition of your EPR Newsletter. Judging from the comments from a great many of you, it is one of the most-appreciated regular features of the Newsletter. We hope you continue to find it useful. But it is useful only if it is current and correct. Please help by letting us know of any errors or incomplete entries that you find and by sending us (e-mail: ierc@uiuc.edu) updates, changes, and suggestions for additions to our list. Also, we always are glad to consider suggestions for new Newsletter features, particularly from those who are willing to do the work to create them.

R. Linn Belford, Editor

## **♦ IES AFFAIRS ♦**

ANNOUNCEMENTS AND REPORTS FROM THE INTER-*NATIONAL EPR SOCIETY* 

## From the President —

This Directory Edition of the Newsletter is one of which we are particularly proud. It circulates to a very high proportion of those engaged in EPR/ESR research in the world, and we hope that those who receive it show it to their colleagues. It is gratifying to our invaluable Sponsors and Advertisers to have their material so efficiently targeted at just the community which uses their equipment and services. And it is an example of a Learned Society acting dispassionately to further and expand interest in its subject worldwide. It was one of the aims of the IES when it was founded to do exactly this, and to put EPR/ESR scientists in touch with one another, and although it is costly for us to supply this edition to members and non- members alike it still seems right to do so. I know of no other Society which provides a comparable service in any other subject area.

At the same time, this service is wholly dependent on the income to the Society and we very much hope that our readers who are not already members will decide to join through this example of what the Newsletter provides. The membership fee is modest (\$30/year) but the income it produces allows the Society to provide the service it does. The Society has expanded in a very satisfying way to encompass the world and is truly international both in its membership and in its decision-making bodies, but it does not yet have the income it needs to expand its activities in the ways that all of us would like to. Those members who I do see at conferences always tell me how much they appreciate the Newsletter in supplying not only essential information, but in creating a feeling of community. Please join and benefit from it yourself!

Keith McLauchlan

## EPR SPECIALIST VIGNETTES

Edited by Arthur Schweiger

The Linear Electric Field Effect in EPR
William B. Mims
226 Rocky Run Rd.
Glen Gardner, NJ 08826, USA

In treatments of the EPR properties of metal ions it has been the standard practice to limit consideration to wave functions which are all of the same parity, for example the 3d-manifold for the iron group, or the 4f manifold for the rare earths. The observed g-values and D-splittings are interpreted as a consequence of the remixing of these wave functions by the even terms in a crystal field, or ligand field, generated by the immediate environment of the metal ion. In such treatments it is usual to discard the odd crystal field terms, (which exist in almost all of the experimental samples reported in the literature), since they are unable to couple states within a given single parity manifold, and can influence the result only in second order perturbation, via state mixing with a manifold of opposite parity, e.g. 4p for the 3d group, or 5d for the 4f group. This second order correction contains the product of two odd crystal field harmonics, yielding an even term, an equivalent even field,1 which can be added to the physically real even terms, from which it cannot be resolved by the methods of conventional EPR. Thus a large fraction of the information regarding site symmetry and bonding-information which has become increasingly important now that the study of simple ionic crystals has made way for the study of more complex centers-remains inaccessible unless standard EPR techniques are developed further.

A method for investigating this odd component has nevertheless been available for several decades. EPR measurements are performed with and without an external electric field applied to the sample. In the language of crystal field theory, this electric field, an additional odd field component, combines in second order with the odd crystal field harmonics already present, to create an increment in the existing equivalent even field. This increment can then be



**Professional Societies & Publications** 

500 Sunnyside Boulevard Woodbury, NY 11797-2999 USA Phone: 1-516-576-2411 Fax: 1-516-576-2481

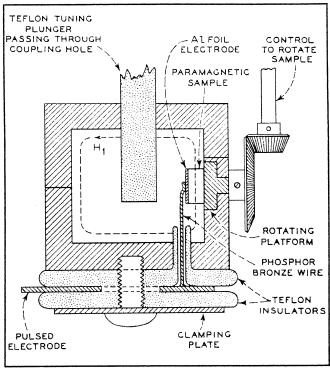


Figure 1: X-Band microwave cavity used in single-crystal experiments on the linear electric field effect.<sup>4</sup> The magnetic field can be applied in any chosen direction with respect to the crystal axes of the sample by a) rotating the platform built into the side of the cavity, and b)rotating the external magnetic field about the apparatus as a whole. The high voltage step is applied to a thin foil electrod mounted on the sample. In the most general case of C<sub>1</sub> point symmetry three separate experiments must be performed with the crystal successively mounted in three mutually perpendicular directions, (e.g. the crystal axes).

manipulated in such a way as to characterise the missing odd crystal field components by changing the magnitude and orientation of the applied electric field.

Unfortunately, the simple direct experiment outlined above only succeeds in a limited number of cases. With fields that can be applied under normal laboratory conditions (e.g.  $10^4$ - $10^5$ V/cm) the shifts in resonance frequency are often no more than the observed inhomogeneous line width. The applied field is barely able to compete with irregularities and strains, or, in the case of some ionic crystals, with the randomly oriented internal electric fields generated by ionic defects.<sup>2</sup> Measurements on a powder or on a frozen solution sample would be virtually impossible by this method.

The difficulty vanishes, and the experiments become easy to perform in a laboratory possessing a pulsed microwave, electron spin echo apparatus. An electric field step is applied to the sample in coincidence with the second pulse of a two-pulse Hahn echo sequence. The sudden shift in resonance frequency, though small, results in a steadily accumulating phase shift that is dramatically evident in the echo signal. For instance, a shift of only 0.25 MHz in the resonance frequency—equivalent to less than 1% of a typical single crystal linewidth—reverses the phase of the echo signal after two microseconds. Echo memory times of this order are commonly found in hydrogen-containing samples, and yet longer times occur in dilute paramagnetic

Publication of the International EPR(ESR) Society

samples that do not contain nuclei with large magnetic moments.

Experimental details can be found in the literature,<sup>3</sup> and it is only necessary to mention here one or two points that might seem problematic. First the cavity. An example of a cavity used in early single crystal experiments is shown in Fig 1.<sup>4</sup> Significant improvements in signal to noise might however be attained by adapting a high filling factor cavity, such as that used in later electric field effect experiments on frozen solutions,<sup>5</sup> for single crystal operation.

Other points to note are the following. Measurements have to be conducted at liquid helium temperatures, not only to ensure an adequate spin lattice relaxation time, but to ensure a long enough phase memory for the echo sequence. The electric field step can be generated by switching a capacitor. No currents, other than the small charging currents for the leads going to the sample, are involved, so a small inexpensive high voltage module is sufficient. The step transition must be fast, but recovery, after the appearance of the echo, can take any amount of time up to the beginning of the next two-pulse sequence. Electrical breakdown need not be a problem for voltages up to about 15KV, provided that the leads are kept clear of helium gas, which is a very poor insulator. For this reason it is best to perform experiments below the helium lambda point in order to avoid bubbling. Liquid helium is an excellent insulator, as also are most samples, including hydrated crystals and frozen aqueous solutions, at low temperatures.

The brief discussion above has been framed in terms of the crystal field theory since this is widely familiar and is used in many textbooks, but for samples that are likely to be of interest nowadays a molecular orbital approach may be more appropriate. This extra elaboration does not affect the overall conditions of the experiment insofar as they are determined by symmetry considerations, but the measurements are likely to have a more specific aim than the mere assignment of a point group to the paramagnetic site. For instance it may be desired to probe the polarisability of a given ligand in a metalloprotein. For this purpose a careful comparison of model calculations with experimental data would be required, and the theoretical challenge could easily exceed that posed by the experiment itself.

Before ending this short note I would like to suggest an experiment that, as far as I know, has not yet been done.

# MICRO-NOW INSTRUMENTS

is a CONTRIBUTOR to

The International EPR Society

EPR spectrometers, components, accessories, and microwave equipment. Model 8320 Magnet Field Controller for replacing older controllers, i.e. Varian Mark I & II and other types. Includes keyboard or controlled by external computer.

8260 N. Elmwood, PO Box 1488, Skokie, IL 60076, USA 5: 708-677-4700. FAX: 708-677-0394

That is, the measurement of the linear electric field effect coefficients for a metal ion center in a single protein crystal<sup>6</sup>. The low spin ferric iron center in cytochrome c would be an obvious choice, since single crystals can be produced fairly easily, it is a two-level system (S'=1/2), the structure is known, and it would be possible to focus on the linear electric field effect and its interpretation without being drawn into other speculations. A study such as this is needed to lay the groundwork, both experimental and theoretical, before embarking on the study of materials that may be more interesting, but are less well characterised. The principal experimental challenge is that of mounting the crystal in a dielectric medium in such a manner that a uniform electric field exists throughout the sample when the voltage step is To a certain extent nature favors the applied. experimentalist here, since at low temperatures the dielectric constants of protein material, and of most of the liquids in which it might be immersed, are more or less the same (i.e. ε≅2). However, certain problems remain, for instance that of constructing a suitable cell to contain the crystal and its ambient medium while it is being cooled down. This technical advance, though small, would open the way for a number of useful applications.

#### REFERENCES:

- 1. A. Kiel, Phys. Rev. 148, 247, (1966).
- 2. W.B. Mims and R.Gillen, Phys. Rev. 148, 438, (1966).
- 3. A comprehensive treatment of the subject is given in W.B. Mims, The Linear Electric Field Effect in

### **ELECTRON SPIN RESONANCE VOLUME 14**

#### NEW VOLUME \* NEW APPROACH

From Volume 14 this series takes a fresh approach to its coverage of the literature in this important area. Its treatment is selective, critical and eminently readable, giving readers an authoritative insight into current trends and developments, in the key areas where ESR is being applied.

#### For further details please contact:

The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF, UK. FAX: 44-223-423429

#### Or in the USA, Mexico and Canada:

CRC Press, Inc., 2000 Corporate Boulevard NW, Boca Raton, FL 33532, USA. 2: 1-407-994-0555.



Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

Paramagnetic Resonance, Clarendon Press, Oxford, 1976. This book has been out of print for some time, but may be available in central libraries. For experimental details of the spin echo method see W.B. Mims, Rev. Sci. Instrum. 45, 1583, (1974).

- 4. W.B. Mims, Phys. Rev. 133, A835, (1964). See Fig. 6.
- 5. Figures showing this cavity appear in both references 3, also in W.B. Mims and J. Peisach, Biochemistry 15, 3863, (1976), and in a number of other places.
- 6. There have been numerous experiments involving the linear electric field effect in non-crystalline protein samples; see e.g. W.B. MIMS, and J. Peisach, chapter I in Advanced EPR, Applications in Biology and Biochemistry, (ed. A.J. Hoff), Elsevier, Amsterdam, 1989. However, the results obtained in these experiments represent an average over many orientations, and much useful physical information is lost.

## A Guest Editorial

by Hal Swartz Dartmouth Medical School, Hanover, NH, USA

#### Lessons for the EPR Community from the 1996 Primary Election Campaign in the USA—

The connections between national politics and the scientific funding process may not be immediately obvious, but I think that there really are some valuable lessons to be drawn, regardless of your country. Many observers of this year's Primary Election process in the USA believe that in their scramble for the nomination to be the Republican candidate for the Presidency, the candidates may have assured the election of the Democratic candidate, Bill Clinton! This is happening because of all of the energy that the various Republican candidates have devoted to pointing out the defects of their rivals. When the actual presidential campaign occurs, the Democrats will have plenty of "data" for pointing out the defects in their opposition.

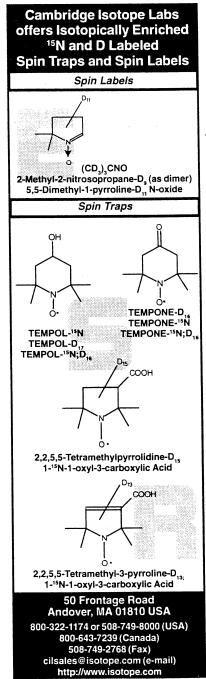
To some extent the Republican candidates (presumably unknowingly) are emulating the EPR community. That is, in too many cases, like them we seem to be devoting too much energy to destructive criticism --in this case in regard to the manuscripts and grant proposals in our own field. And we do not put enough energy into pointing out the strong points and fundamental value of the approaches that are being put forth and to making constructive suggestions as to how the proposals/papers can be improved. As a consequence for the EPR community, too often, the well-based criticisms tend to dominate the decisions that are made, and the grants do not get funded and the papers do not get accepted! While at first glance this habit of strong critical review of our peers may seem to be the intellectually honest and proper thing to do, I believe that closer analysis indicates that this is not necessarily the case. Often reviews of the EPR aspects of proposals/manuscripts are sought by individuals or committees who do not feel that they have the technical

background to make an accurate assessment of the EPR aspects and they are seeking information on the technical competence and significance of the proposal or manuscript. Usually they neither seek nor need an evaluation of whether this is the best possible way in the world to do the EPR experiment or if the authors are going to do it the way that you would have done it.

I offer the following specific suggestions on how you might consider approaching the review of papers and proposals in order to provide intellectually honest reviews that also offer an opportunity to advance the field.

In regard to papers, the aim should be to try to facilitate

publication the of papers strong that highlight the scientific value of the use of EPR techniques. Excellent papers should praised warmly and minor defects should be noted to help authors improve an already highly acceptable paper. If one regards a manuscript as clearly beyond redemption, the criticism and recommendation not to publish it should be made in as polite and constructive manner as possible, and should include specific suggestions as to the shortcomings and how to avoid the perceived fatal flaws. Where the paper seems potentially salvageable. important to provide a strong positive message to the editor on the potential worth of the paper and to provide the author with a detailed but fair critique as to what is wrong and, where appropriate, to indicate means to remedy the defects. That is, one aim of the review process should be to keep the paper in a position where,



Publication of the International EPR(ESR) Society

## JEOL USA, Inc.

Manufacturer of CW Electron Spin Resonance Spectrometers Featuring a Compact Design with High Sensitivity and High Reliability

11 Dearborn Road, Peabody, MA 01960, USA Phone: 1-508-535-5900; FAX: 1-508-536-2205 E-mail: dipas@jeol.com

sufficiently improved, it will become publishable; sometimes, especially where the editor is not closely involved in EPR, a critique may be misread as indicating that the paper is unlikely to be able to be improved sufficiently to be published.

In regards to grant proposals, there are some very important additional considerations. The failure to get a research grant funded in a timely manner can have serious implications for the progress of the career of the applicant, so it is important to differentiate between: 1. defects which make the proposed research unsupportable and therefore the proposal needs to be rewritten and resubmitted (which in the USA usually means at least a 9 month delay in the possible starting time for funding); and 2. a problem which can be resolved by a reasonable change in approach. In the second case it is very important to stress the positive parts of the research proposal and its importance, and to discuss the weaknesses as potential and to indicate how, without major changes, the research can be improved. For example, I recently reviewed a proposal for collaborative research with an EPR laboratory in which the write-up of the EPR portion was not very sophisticated and not likely to accomplish the goals of the research. The EPR group which was to be involved, however, was very competent and experienced in the area of proposed research and very likely to carry out the experiments properly, even though they were not described well in the proposal. It seemed to me that there was little to be gained by strong criticism which would have been likely to result in the necessity for revision and resubmission. Instead I pointed out the potential value of EPR for achieving the goals of the research and the high competence of the collaborating EPR group and said that while the description of the proposed experiments was lacking in some significant aspects, the collaborating EPR group was virtually certain to carry out the studies with the techniques and level that was needed and therefore I enthusiastically supported the research. I was able to do this because I genuinely believed what I said. I think that latter is key-- we should not support research just because it involves our EPR colleagues but we should look at what is likely to be done and should not focus exclusively on the details of the presentation.

In the long run we all benefit from excellent research done using EPR techniques; we should focus our input towards this goal and not get caught up in the game of showing how knowledgeable we think that we are. And we should recognize that our non-EPR colleagues may have a high degree of respect for us and therefore our words of criticism may have considerable weight and therefore should be applied prudently and constructively!

# Building The Perfect Beast

by Chris Bender NIH Biotechnology Resource for Pulsed EPR bender@spin.aecom.yu.edu

#### 1. Preamble

One of the marvelous little gadgets that Bill Blumberg built is an optoelectronic 'mouse' that is used to vary the timing parameters on our spectrometer. The device consists of an optocontroller (described further below) and a bank of contact switches. The operator presses a given switch, which passes an interrupt to the 6505 microprocessor and specifies an address on the IEEE interface. With the switch closed, the pulses generated by the optocontroller step the specified delay generator incrementally in either direction.

The problem with mice is that some people seem to think that they are used as an object to be rapped on the lab bench in order to get the computer's attention, and I often find myself replacing parts that weaken with repeated impact (multistrand cables and their crimp connectors in particular). Keyboards are more robust, and so I decided to simulate Blumberg's mouse by writing program code that passes control to the keypad editor adjacent to the alphanumeric keys. John McCracken at one time suggested a rollerball device similar to the Atari game controller, but my feeling was that the latter device is small enough to be damaged.

#### 2. The Blumberg Mouse

The schematic diagram for the Blumberg mouse is illustrated in Figure 1. The computer interface is made via a 16-conductor ribbon cable that connects to a custom board. Eight switches constitute a bank, and the active switch is designated by making contact. Specifically, the switches are connected to a +5V bus bar, and therefore a closed switch is indicated by a logical HI. This logical HI is, in turn, used to select the active address in computer.

Depressing any button passes an IRQ (interrupt request to the computer). The Apple II's 6502 processor has two hardware and one software interrupts. An IRQ is essentially a status flag that is polled on each clock cycle; if flagged positively, the CPU stores its current register in memory, loads a status register, and proceeds with some specified procedure. The logical state of the seven member switch array, that is, a message of 0's and a single 1, would constitute the contents of a status register; in other words, it can identify the switch that signifies a request and route the procedure accordingly. The advantage of IRQs is that it permits one to handle responses to asynchronous events, and

ordinarily one sticks a specialized chip called a Programmable Interface Adapter (PIA) as a buffer between the CPU and outside world (note 1).

Nimble fingers are meanwhile turning the knob of the optical controller, which puts out 200 pulses per rotation on two channels. If rotation of the knob is clockwise, the pulse on output channel A precedes the pulse on channel B by

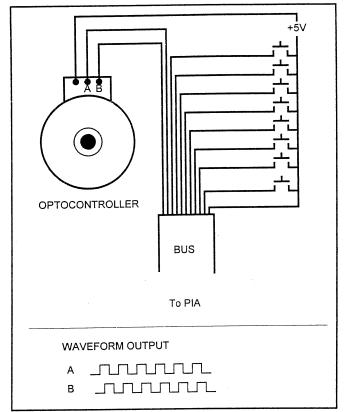


Figure 1: Wiring diagram of the Blumberg 'mouse'. A 200 pulse per rotation optocontroller supplies waveforms on two channels, and a switch bank encodes the 8-bit address of the device that is updated by the pulse train. A board occupying a slot on the Apple II motherboard contains the hardware interface to the mouse and the devices (GPIB-style, a now obsolete version of the IEEE-488 standard).

approximately 90°, and vice versa (Figure 1, bottom). The optical encoder itself is a bit like those old color wheel lamps that were popular for shining on aluminum Christmas trees in the 1960s, or, for those of you who missed the sixties (perhaps too the phenomenon was unique to the Bronx), an optical chopper that is used in optical labs to modulate a photoeffect. A lamp of some sort (LED) is placed on one side of a wheel and (in this case) two photodiodes are positioned on the opposite side of the wheel (Figure 2). The wheel has two overlapping slots cut into it so that the photodiodes are illuminated independently, and the pattern of those slots will determine whether the pulses are separate or in quadrature (as depicted in Figure 2).

The unit described in Figure 2 is actually an oversimplification. I dissected a dead encoder that features (a lot of) small slits cut along the radius of the disk. There are two diodes and detector pairs and two rows of these slits.

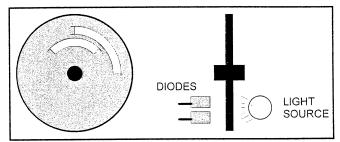


Figure 2: Simple representation of an optical encoder. Two slits are cut into a wheel and allow illumination of two photodiodes at offset times.

There is also a stationary foil that has two pairs of three slits on it. In other words, there are two diodes to generate the light and what looks like four detectors arranged in pairs and separated by about  $20^{\circ}$ . I would guess this duplication (the shutters open simultaneously) constitutes a discriminator to avoid false positive readings. The slits on the flywheel are coincident; the slits on the stationary wheel are offset.

The desired effect of the optocontroller is to increment or decrement the pulse generator depending on which direction the encoder's shaft is turned, so a discriminator is required. The spec sheet indicates that the directionality is manifest in the quadrature of the pulses on channels A and B. One could take various strategies, for example, a two counting channel with a facility for 'blanking', or a single counting channel and a logical HI/LO to designate add or subtract. One way to do the former is use a pair of JK flip-flops with the encoder's A and B inputs passed to the clock input of each flip-flop (two are on a 7473 chip); J and K inputs are both HI. If you then pass the A channel also to the B flip-flop's clear and the B channel to the A flip-flop clear, the B flip-flop will not trigger when the A pulse arrives first, and vice versa. The flip-flop triggers on the falling edge and if the clear is held LO while the trigger arrives, then the event is missed.

Blumberg's method of handling the event/direction discrimination is more sophisticated and is tied to the programmable PIA. At this level of hardware manipulation, program code is written in 6502 instruction set, and for those not familiar with such programming, the computer is broken down into a sequence of addresses that can be occupied by an 8 bit word. There is an active stack of 5 or so registers that are used as a workspace for manipulating numbers. My delay generator, for example, resides permanently at some address

## /// 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

Publication of the International EPR(ESR) Society

in the Apple II computer's memory; I can change this only by altering Blumberg's original instruction set code and parameter tables that accompany it (for a good intro to writing instruction set code and procedural details, see the four books listed in the bibliography). At the address corresponding to my delay generator is a number or word that (presumably) reflects the current status of the instrument. The word corresponds to the delay time set on the generator. Each pulse passed to the computer from the mouse increments or decrements (by integer value 1) the integer word that is located at the specified address.

The instruction set program therefore works as follows. An interrupt request is signaled by depressing a switch on the 'mouse'. The IRQ comes as an 8 bit word that is used by logical statements to assign a device address (there is provision for four delay generators and four servo motors). Whatever word is located at the specified address is recalled to the register and either incremented or decremented by one, depending on the logical sequence of pulse inputs from channels A and B.

#### 3. The Keypad 'Mouse'

The architecture of the Blumberg mouse software and control of peripherals on the Apple II is very fundamental and is written in microprocessor chip instruction set that is linked directly to the hardware logic. When working with higher level languages and commercial hardware, you are doing the same thing, but someone has done the painstaking work of writing the instruction set code (usually proprietary and loaded onto ROM chips where you never see them) for the hardware and written a higher level language code that calls these instruction set programs. The keyboard is just such a device; since I really only need to send a pulse to increment the delay generator (I have abandoned the servo motors and their promise of automatic seat height adjustment - actually, Blumberg, I believe, envisioned servo-driven tuners), depressing specific keys will provide me with the same, albeit less elegant, function as Blumberg's mouse.

The editor keypad features four (or more) 'arrow keys' that are normally used to mover the cursor around a text file. The spectrometer features three Berkeley Nucleonic programmable delay generators, designated D0, D1, and D2. The keypad arrows provide an intuitive function according to the following 'code':

## SCIENTIFIC SOFTWARE SERVICES

P.O. Box 406 Normal, IL 61761-0406 USA Voice/Fax: 309-829-9257

Contributor to the International EPR Society

Cost-effective EPR data acquisition, simulation, deconvolution, and imaging software for ALL EPR spectrometers.

Free DEMOs available.

CALL for further information and pricing
Web site: http://www.wwnet.com/~sss/

 $[\rightarrow]$  - increment delay by 1.

[ - decrement delay by 1.

[ † ] - change active delay generator, positive permutation (D0-D1-D2-D0 . . .).

[  $\downarrow$  ] - change active delay generator, negative permutation (D2-D1-D0-D2 . . . ).

One does not want to be left with the only step size being 1 ns, and therefore the modifier keys <rshift>, <lshift> are used to designate multipliers of 10 and 100, respectively. Other functions can be added as desired from other combinations of keypad keys and modifiers. For example, I use the <HOME> key to reset the timing delays to their initial values after collecting an echo modulation.

I use a simple logic statement to pass control of the spectrometer program to the keypad editor.

while (!key\_ctrl()); or while (key\_ctrl()); The function  $key_ctrl()$  returns a positive number or 0 depending on what editor key is hit, so if I am incrementing the generators I want the absolute value of the step to be a sign that the loop should continue. I specify a 0 as a signal to exit, and this terminates the implicit while loop. Here is a simple example that demonstrates how the thing works: #include <stdio.h>

main()
{
 extern int sniff();
 while ( sniff() ); \\ this will remain in while condition until
 sniff returns 0
 printf ("\nOK, show's over.\n" );

# NIKKISO Co., Ltd. SUMITOMO SPECIAL METALS Co., Ltd. SUPPORTER of the International EPR Society

Innovative Portable EPR Spectrometer with a built-in 32 bit computer (ES-10)

Frequency: 9.4 Ghz

Sensitivity: 2\*10<sup>10</sup> spins/0.1 mT

Resolution: 6\*10<sup>-5</sup>

Size: 500x500x230 mm

Weight: 25 kg

Magnet: NEOMAX-40

SUMITOMO SPECIAL METALS AMERICA, Inc. (Tel)310-378-7886, (Fax)310-378-0108

```
exit ( 0 );
}
int sniff ( )
{
  int s;
  printf( "\nEnter some digit: ");
  scanf( "%d", &s );
  return s;
}
```

The program *main()* passes control to function *sniff()* until the hapless user enters a zero that is then recognized by the while statement as a logical and concludes. I do the same thing with the *key\_ctrl()* function; a miscue (unrecognized keypad entry) or <ctrl> will return zero and disengage the while statement, allowing the user to return to the spectrometer control *main()*.

My function  $key\_ctrl()$  is modified from a Borland example program that illustrates a function called bioskey(). The function bioskey() is a C version of the familiar DOS function that controls and encodes keyboard input. The code is fairly straightforward and listed at the end of this article, but its function is to grab a keyboard entry, identify the key pressed and any modifier, and perform a function based on specified flags. The function  $update\_gen()$  represent a call to the board specific functions that come with a National Instruments IEEE interface card; the other functions  $incr\_gen()$  and  $decr\_gen()$  are cheesy little functions that permute the logic that designates the active delay generator.

```
Here is simplified code for <code>key_ctrl()</code>
int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code> int <code>key_ctrl()</code>
```

```
if ( modifier & RIGHT ) multiplier = 10;
if ( modifier & LEFT ) multiplier = 100;
if ( modifier & CTRL ) return 0;
if ( key == RARROW ) s = s + 1 * multiplier;
if ( key == LARROW ) s = s - 1 * multiplier;
update_gen( de, s, time );
return s;
}
```

For the above code to work, it needs a statement while (s = key\_ctrl(s))

to cycle it; the boldface constants are hex integers for key identification. This function becomes more complicated when I want to use other keypad keys and logic to change the active delay generator etc. You can test the above to see how it works as follows:

```
int s = 0;
while ( s = key_ctrl( s ) ) printf( " The current value of s is
%d\n", s );
```

### Bibliographic Material:

Findley, R., 1979, 6502 Software Gourmet Guide and Cookbook, SCELBI Publications: Elmwood.

deJong, M.L., 1980, Programming and Interfacing the 6502, with Experiments, Howard Sams: Indianapolis.

Leventhal, L.A., 1979, 6502 Assembly Language Programming, OSBORNE/McGraw-Hill: Berkeley.

Zaks, R., 1979, 6502 Applications Book, SYBEX: Berkeley.

NOTE 1: C-program prototypes were mailed with this Newsletter article that illustrate the principles described in this column. The program runs on a PC clone (written and tested on a Gateway 2000) off DOS. I have left out the National Instruments functions (in order to avoid nasty legal 'incidents'), but the program provides a naive and simplistic way to interface a homebuilt spectrometer; there is also a bunch of demos that take you through isolated routines of the program, and one that simulates "the Einstein experience" (up to a point; there's nothing quite like being here). The algorithm that I used deviates slightly from the specific code described in this article because I needed to be able to pass parameters among the various program 'functions'; the rationale is explained in the program documentation, but in short, I found it much simpler to set up a parameter table as

## **CPI Sets the Standard for EPR Klystrons**

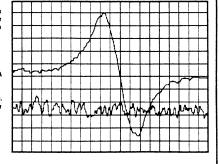
CPI Replacement Klystrons deliver:

- Optimum application flexibility Long Life
- Reliable performance, low noise New warranty
- X band for Century Series, E lines, plus Q band
   Now available directly from CPI. For more information call
   CPI at 1-800-843-8780 or 415-846-3188 from outside the U.S.



formerly a division of Varian @

taken with a Varian weak pitch sample in a TE192 cavity under the conditions specified in the Varian E Line Series unmodified (E102/E109 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 .843 multiplication factor. Without the multiplication factor, the signal to noise would be 386:1.



Publication of the International EPR(ESR) Society

a global variable and use nested while statements instead of function calls to route the program through its duties.

## FROM EPR CENTERS

#### A National Service Centre for Continuous Wave Variable Temperature Electron Paramagnetic Resonance Spectroscopy

Service Manager: Dr. F.E. Mabbs Chemistry Dept., Univ. Manchester

As part of a grant to the Chemistry Department of the University of Manchester, EPSRC have funded a National Service for Continuous Wave Electron Paramagnetic Resonance (c.w.EPR) Spectroscopy. The Service, which will occupy 75% of the instrument time, will be of interest to Chemists and Biological, Medicinal, Materials Scientists. Use of the Service will be in accordance with the following order of priority: (i) EPSRC grant holders or workers eligible for a Council grant, Council supported students, and Council staff for Council approved use; (ii) users who are eligible for support from one of the other Research Councils; (iii) all other users. There will be no charge to holders of Research Council grant-holders or to workers eligible for Research Council grants. However, users may have to provide specialist materials or equipment. The Service is based on a completely new Bruker ESP300E-13/15Z spectrometer system. The facilities available are (i) L-band (ca. 1 GHZ), S-band (ca. 3 GHZ), X-band (ca. 9 GHZ), Kband (ca. 25 GHZ), and Q-band (ca. 35 GHZ) microwave frequencies, with a dual mode resonator at X-band; (ii) magnetic fields from 0 to 1.85 Tesla; (iii) temperature range 4.2 to 700K; (iv) spectrum simulation for single and multiple unpaired electron systems.

The service offered will be at a number of different levels of sophistication:

- Level 1. Single frequency at temperatures in the range 100-700K on solutions and powders.
- <u>Level 2</u>. Multiple frequency measurements on solutions and powders in the temperature range 100-700K.
- <u>Level 3</u>. As in level 2 but with spectrum simulation and assistance with interpretation.
- <u>Level 4</u>. As in level 3 but with measurements at temperatures below 100K.
- Level 5. Single crystal measurements.
- <u>Level 6</u>. Specialist measurements by arrangement with the applicant

Users of the Service, particularly research students, are encouraged to be present when their samples are run. Limited funds are available to support this, but we expect these to be used when researchers need to be present for several days at a time.



Applications to use the Service must be made on the application form, available from Dr. F.E. Mabbs, EPSRC c.w.EPR Service Manager, Chemistry Department, University of Manchester, Manchester, M13 9PL. You are advised to consult Dr. F.E. Mabbs (\* 44-161-275-4650; FAX: 44-161-275-4582; e-mail: frank.mabbs@man.ac.uk) or Dr. D. Collison (\* 44-161-275-4660) before making an application.

## **NOTICES OF MEETINGS**

28th CONGRESS AMPÈRE on MAGNETIC RESONANCE, University of Kent, Canterbury, UK, September 1-6, 1996.

Extensive information about this conference can be found in Vol. 7, No. 4 of the *EPR Newsletter*. More detailed information can be obtained by contacting The Secretariat, 28th Congress Ampère, The Physics Laboratory, University of Canterbury, Kent CT2 7NR, UK; **2**: 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.

Some details about this conference, with a partial list of invited speakers, can be found in Vol. 7 No. 4 of the *EPR Newsletter*. For further information please contact Assoc. Prof. Hanna B. Ambroz, Inst. Nuclear Chemistry & Technology, ul.Dorodna 16, 03-195 Warsaw, Poland. **3**: 48-22-11-23-47, FAX: 48-22-11-15-32.

#### 28TH SOUTHEASTERN MAGNETIC RESONANCE CONFERENCE, Univ. Alabama, Tuscaloosa, Alabama, USA, October 9-11, 1996.

Featuring EPR, NMR and related techniques. Martin Bakker, **2**: 1-205-348-9116, e-mail: bakker@uatvm.ua.edu. WWW: http://www.as.ua.edu/chemistry/

#### 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.

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

The Conference will be held at the Cultural Centre 'Tulio Febres Cordero', Merida. Inquiries should be sent as soon as possible to Sue Owen, Conference Secretariat, BIOSim 96, Wessex Inst. Technology, Ashurst Lodge, Ashurst, Southampton, SO40 7AA, UK; **3**: 44-1703-293223; FAX: 44-1703-292853; E-mail: cmi@uk.ac.rl.ib; Intl. E-mail: cmi@ib.rl.ac.uk.

## OXYGEN '96, Eden Roc Resort & Spa, Miami Beach, Florida, USA, November 21-25, 1996.

Special events include the "Biological ESR Workshop" on November 21, and a "Sunrise Free Radical School" each morning. For information, contact Oxygen '96 c/o The Oxygen Society, 74 New Montgomery, Suite 230, San Francisco, CA 94105-3411, USA. **2**: 1-415-546-3124.

\*More information about the Biological ESR Workshop at Oxygen '96 is available at the end of the Meeting Notices, (page 12).

# 1st ASIA-PACIFIC EPR/ESR SYMPOSIUM, January 20-24, 1997, Hong Kong.

The aim of this symposium is to bring state-of-the-art knowledge of EPR and related magnetic resonance techniques to Hong Kong and southern China. The Symposium will constitute an unique opportunity to bring together active researchers, leading world experts, and potential users of EPR techniques. The Symposium, although aimed primarily at Asia-Pacific countries, is open to participants from all over the world.

In order to promote and facilitate collaboration among EPR/ESR researchers and users from the Asia-Pacific region, during the Symposium a special session for the Inaugural Meeting of the Asia-Pacific EPR/ESR Society (APES) will be held. The establishment of the Regional EPR/ESR Society, to be affiliated with the International EPR(ESR) Society, has full support of the parent Society. Areas of interest include:

- mineralogy including gemmology
- polymers
- EPR dosimetry and dating
- environmental science and protection
- · fossil fuels
- medical applications
- biological and photosynthetic systems
- semiconductors
- magnetic materials
- high temperature superconductors
- ferroelectrics and optoelectronic materials
- new developments in EPR and related technniques

Contributions will be in the category of either invited papers for plenary sessions or of contributed papers for either parallel topical sessions or poster sessions. Time for presentations at the plenary and topical sessions includes discussion. The Symposium language will be English. Four parallel topical sessions encompassing the following fields are planned:

- · biology, life and medical sciences,
- · chemistry, earth and environmental sciences,
- · physics and materials science
- new developments and cross-disciplinary areas.

Abstracts of contributed papers will be refereed by the Scientific Programme Subcommittee with the help of external

## OXFORD INSTRUMENTS

Supporter of the International EPR Society

#### EPR Cryostats

Cryostats designed specifically for X and Q band EPR experiments

- · Helium and nitrogen cooled version available
- Efficient use of cryogen
- Temperature range 1.8 300 K standard (higher temperatures available on request)
- Temperature stability ± 0.1 K

### Teslatron<sup>H</sup>

Compact high homogeneity Teslatron systems for high field EPR and other applications

- · Automated magnetic field and temperature control
- Applied fields from 7 to 20 Tesla
- 10 ppm and 1 ppm homogeneities available
- Integration of experiments using National Instruments LabVIEW<sup>®</sup>
- Available in ultra low-loss cryostats for greatest cryogen efficiency
- Choice of room temperature access or integral variable temperature insert

Call us now for copies of our Teslatron<sup>H</sup> and ESR product guides

# Oxford Instruments Scientific Research Division Research Instruments

130A Baker Avenue Concord, MA 01742 USA

Tel: 1-508-369-9933 Fax: 1-508-369-6616 E-mail: epr@oxinst.co.uk



reviewers if necessary. A book of abstracts will be distributed to participants at registration.

For further information, contact the Symposium Secretariat, Dr. S.K. Wong, (\*: 852-2788-7662; e-mail: apskwong@cityu.edu.hk) or Prof. Czeslaw Rudowicz, Chairman, Dept. of Physics and Materials Science, City Univ. of Hong Kong, 83 Tat Chee Ave., Kowloon, Hong Kong (\*: 852-2788-7787; FAX: 852-2788-7830; e-mail: apsper@cityu.edu.hk). Information on the Symposium can also be found on the WWW home page: http://www.CityU.edu.ku/AP/.

Publication of the International EPR(ESR) Society

30th ANNUAL INTERNATIONAL MEETING: "ESR SPECTROSCOPY OF RADICALS IN ORGANIC AND BIOLOGICAL SYSTEMS" in conjunction with the 5TH INTERNATIONAL SYMPOSIUM ON SPIN TRAPPING: "APPLICATIONS IN CHEMISTRY, BIOLOGY AND MEDICINE", April 6-10, 1997, Lancaster, UK.

The 30th meeting of the ESR Group of the Royal Society of Chemistry, London will celebrate 29 consecutive years of International meetings on the topic of Electron Spin Resonance Spectroscopy. The meeting will be held at The Univ. of Lancaster, in conjunction with the 5th International Meeting on Spin Trapping. The Conference opens with a reception and dinner on Sunday evening and closes after lunch on Thursday. The organisers have pleasure in extending a cordial invitation to all persons interested in ESR spectroscopy in Chemistry and Biology to attend. Accommodation will be in individual rooms in a Hall of Residence on the campus, where the lectures will take place.

Registration forms will be sent out in October to all who have indicated an interest in the Conference. The circular may be viewed on the internet at the following address:

http://www.cf.ac.uk/uwcc/chemy/rowlandscc/conf.html

Scientific Programme: the following have accepted invitations to present lectures: Dr. A. Alberti (C.N.R. Bologna) Title to be announced; Prof. M. Brustolon (Univ. Padua) Pulsed EPR and Molecular Motions in Solids; Dr. M.J. Davies (The Heart Research Inst., Sydney) EPR Spin Trapping Studies on the Degradation of Biological Macromolecules; Dr. G. Gescheidt (Univ. Basel) Radial Ion Pairs: from Geometry to Reactivity; Dr. D.G. Gillies (Univ. Surrey) Radiofrequency Spectroscopy and Imaging; Dr. K.A. McLauchlan (Univ. Oxford) The Bruker Lecture: Physical Chemistry through Electron Spin Polarization; Dr. D. Marsh (Max Planck Inst. Gottingen) Non-Linear ESR Methods for Spin Label Studies in Biological Systems; Dr. R. Mason (NIEHS, N. Carolina) Spin Trapping from Chemistry to Toxicology; Prof. K. Möbius (Freie Univ Berlin) Steady-State and Time-Resolved High-Field Photobiology EPR/ENDOR Experiments in Photochemistry; Prof. A. Rassat (Ecole Normale Supérieure Paris) Magentic Properties of Nitroxide Biradicals; Prof. H. Swartz (Dartmouth Medical School) EPR(ESR) Studies in

## WILMAD GLASS Co.

is a CONTRIBUTOR

to the International EPR Society

"Serving the Spectroscopic Aftermarket"

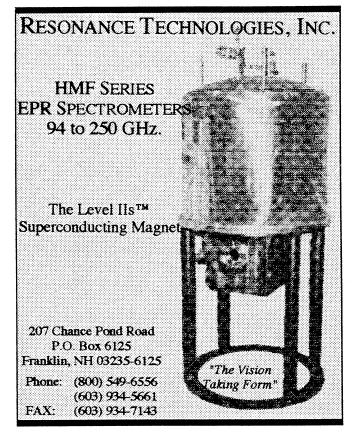
EPR Glassware/Quartzware. Sample cells. Dewars.

Address:

Route 40 & Oak Rd. Buena, NJ 08310, USA

Phone/FAX:

609-697-3000 / 609-697-0536



vivo: Results, Opportunities and Challenges; Prof. A. Tomasi (Univ. Modena) Nitrone- and Heme-Trapping of Free Radicals in Biological Model Systems.

For more information, contact Dr. C.C. Rowlands (Secretary of the Committee of the ESR Group, Royal Society of Chemistry) Dept. of Chemistry, Univ. Wales, Cardiff, P.O. Box 912 Cardiff CF1 3TB, UK; e-mail: saccr@cardiff.ac.uk.

FIFTH INTERNATIONAL WORKSHOP ON ELECTRON MAGNETIC RESONANCE OF DISORDERED SYSTEMS (EMARDIS) and 2nd INTERNATIONAL SEMINAR ON APPLIED EPR, June 1997, Sophia, Bulgaria.

Extensive information about these meetings can be found in the previous issue of the *EPR Newsletter* (Vol. 7 No. 4).

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; \$\frac{113}{2}\$: 3592-713-2546 or -3917; telex: 22729 echban, e-mail: NDYEPR@BGEARN.ACAD.BG

THIRD EUROPEAN ESR MEETING, August 25-29, 1997, Leipzig, Germany.

The title of this meeting is "Modern Aspects of Structure and Dynamic Investigations of Paramagnetic Systems by

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

EPR". A list of topics for this meeting can be found in the EPR Newsletter, Vol. 7 No. 4.

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; **3**: 49-341-235-2630; FAX: 49-341-235-2317; E-Mail: beckert@mpgag.uni-leipzig.de

FIFTH INTERNATIONAL CONFERENCE ON SPIN CHEMISTRY, October 26-31, 1997, Jerusalem, Israel.

An official circular will be available shortly. For more information please contact Haim Levanon, Dept. Physical Chemistry, The Hebrew University, Jerusalem, 91904 ISRAEL. 2: 972-2-658-5544; FAX: 972-2-618-033; e-mail: levanon@vms.huji.ac.il.

\*More Information on the BIOLOGICAL ELECTRON SPIN RESONANCE WORKSHOP, a one-day workshop presented on Thursday, November 21, 1996 at OXYGEN '96:

Lectures by Garry R. Buettner, Art Heiss, Colin F. Chignell, Ronald P. Mason, Walee Chamulitrat, B. Kalayanaraman, Ralph Weber, Harold M. Swartz, Jay L. Zweier.

For more information about this workshop, including news about lecture topics, call The Oxygen Society; **2**: 1-415-546-3124.

# POSITIONS AVAILABLE & WANTED

## **POSITIONS AVAILABLE**

Postdoctoral Research Associates/Sabbatical Visitors. We have opportunities in our research group for postdoctoral research associates and sabbatical visitors. There are 3 immediate openings for persons with strong biochemical background or strong preparation in EPR instrumentation and good practical skills.

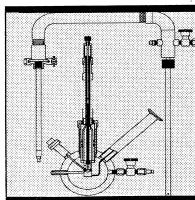
One project involves site-directed mutagenesis of myoglobin and the preparation of spin-labeled myoglobin containing various metals substituted in the porphyrin. Measurement of distances via the impact of paramagnetic metals on the relaxation time of the spin label is the goal of this project. This position requires a person with strong biochemical background including skill in protein purification and mutagenesis. Knowledge of EPR is not required for this position, although the individual will have the opportunity to learn about EPR.

A second project involves preparation of spin-labeled carbonic anhydrase and the study of protein folding by EPR. This position requires a person with strong biochemical background and skill in protein purification. Knowledge of EPR is not required for this position, although the individual will have the opportunity to learn about EPR.

A third project involves design and construction of EPR resonators and associated parts of the spectrometer, and testing practical applications of new resonators for measurement of relaxation times, ESEEM, and other pulse sequences. This project requires a person with strong preparation in EPR instrumentation and good practical skills. For this project an ability to use, or learn to use, microwave simulation programs such as HP's HFSS will be a plus. This research associate will work closely with us and with Richard Quine and Dr. George Rinard from the Engineering Department.

Please contact Gareth or Sandra Eaton for further information. Dept. Chemistry and Biochemistry, Univ. of Denver, Denver, CO 80208 USA; **\$\sigma\$**: 303-871-2980, or 303-871-3102; FAX: 303-871-2254; e-mail: geaton@du.edu or seaton@du.edu; www: http://www.du.edu/~geaton or http://www.du.edu/~seaton.

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

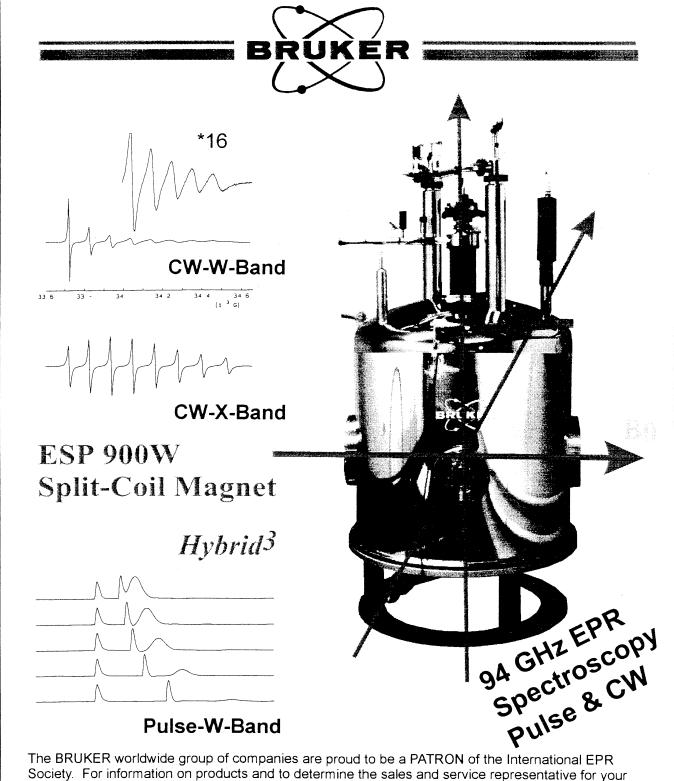


### EPR/ENDOR CRYOSTATS

Uses Liquid helium or nitrogen -- Push or Pull Operation
Plus, our replacement transfer line for your existing cryostat can Save you up to 50% on you liquid helium costs - Cooldown samples faster
- Lower your terminal temperature and Increase reliability!
Call or fax us for additional information:

CRYO Industries of America, Inc., 11 Industrial Way, Atkinson, NH 03811 Tel: (603)893-2060, Fax: (603)893-5278

Publication of the International EPR(ESR) Society



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: 49-721-51 61-141; FAX: 49-721-51 61-237; email: epr\_sales@bruker.de. In the USA, contact Dr. Arthur Heiss, BRUKER Instruments, Inc., 19 Fortune Drive, Manning Park, Billerica, MA 01821. Telephone: 508-663-7406; FAX: 508-670-8851; email: ahh@bruker.com.

PAID ADVERTISEMENT

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.

### 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 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; **3**: 1-713-743-3251; FAX: 1-713-743-2709; e-mail: wasowicz@jetson.uh.edu or

# EQUIPMENT & SUPPLIES EXCHANGE

#### KLYSTRONS AVAILABLE

wasowicz@orange.ichtj.waw.pl.

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; **2**/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; **2**: 1-864-294-3372; FAX: 1-864-294-3559; e-mail: knight lon/furman@furman.edu.

#### **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; 2: 1-303-871-2419.

#### FOR SALE: VARIAN SYSTEM

Micro-Now Instruments presently has available:

 a VARIAN Century series console with field dial regulator, high and low frequency modulation units, Models E207 and E204, oscilloscope and digital drive recorder

## **GMW** Associates

- Laboratory Electromagnets & Power Supplies
- Precision Hall Effect Teslameters
- Digital NMR Teslameters
- Digital Voltage Integrators
- Precision Current Transducers

Specializing in Magnetic Measurements and Electromagnet Systems PO Box 2578, Redwood City, CA 94064 USA. Tel (415)802-8292 Fax (415) 802-8298

Publication of the International EPR(ESR) Society

- 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
- 7) VARIAN V4500-41A low/high power microwave bridge with new klystron—excellent condition
- 8) X-band DEWAR probe with tuner and stainless steel waveguide
- 9) VARIAN E110 Q-band bridge with cavity
- 10) 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**

#### WEIL HONORED AT CONVOCATION

We have received word that our well-known colleague Dr. John A. Weil, Professor of Chemistry, has been honored by the University of Saskatchewan at Saskatoon as its Outstanding Researcher for 1996. Prof. Weil is a charter member and Council Member of the International EPR Society.

He is famous for his many contributions to EPR as a high-precision measurement science and especially for his extensive investigations of magnetic centers in crystalline quartz. The award was presented at the May 1996 University Convocation in Saskatoon. Congratulations, John!

#### 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 1,400+ 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.

#### 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.

#### UPDATED E-MAIL ADDRESSES ON WWW

Since e-mail has become the popular means of communication for so many of us, having the correct e-mail address for the people we need to contact is vital. While the directory issue published each year helps, we receive changes almost every day as e-mail systems are constantly being upgraded and expanded. To assist in communications among EPR researchers, we are going to put e-mail addresses on the IES WWW. This list will be updated each month, so you will be able to find addresses for many people whose old e-mail does not work. Please check your own e-mail address on the Web to see if we have the correct one. If not, send your new or corrected one to ierc@uiuc.edu

## Summit Technology Inc.

8827 Osceola Ave.

Morton Grove, IL 60053

Phone: 1 800 735 6327 / 847 470 1638

Fax: 847 470 1562

Email: 73173.1415@compuserve.com

http://ourworld.compuserve.com/homepages/summit1

## Supporter of the International EPR Society

- EPR Spectrometers
- Microwave Bridges
- Magnetic Field Controllers
- Variable Temperature Controllers
- Spectrometer Repair and Modification
- · Visit our home page on the world wide web

Volume 8, Number 2

Page 1

Summer/Fall, 1996

## ALIKHOV RECEIVES THE GOLD MEDAL FROM INTERNATIONAL EPR (ESR) SOCIETY

On July 22, the 1996 Gold Medal of the International EPR (ESR) Society was awarded to Professor Kev Minullinovich Salikhov during the International EPR Symposium in Denver.

The occasion was marked by a Gold Medal Award Session that featured a personal presentation from Prof. Keith McLauchlan, President of the Society, an award address by Professor Salikhov entitled "Theoretical Approach to the Analysis of Arbitrary Pulses in EPR Experiments" (which was coauthored by Prof. Jack H. Freed, Cornell), and lectures by both Prof. Keith A. McLauchlan, Oxford, and Prof. James S. Hyde, Medical College of Wisconsin. In addition, there was a gala banquet on the next evening to honor the Gold Medalist as well as the Silver Medalists and others. Attendees were



IES Gold Medalist Kev Salikhov (right) accepts the prize from IES President Keith McLauchlan during the International EPR Symposium in Denver, July, 1996.

treated to some personal reminescences and stories about Kev Salikhov by others, including Larry Kevan and Jim Hyde. To celebrate this Gold Medal Award, Jim presented Kev with a real gold medallion as a personal gift from Karen and Jim Hyde. Kev responded to the stories in his modest way, and treated us all to a Tatar song. It was a beautiful occasion!

- Editor: R. Linn Belford, Urbana, IL
- •Assistant Editor, Becky Gallivan, Urbana, IL
- Typography: Martha Moore, Urbana, IL.
- This, the official newsletter of the International EPR(ESR) Society, is supported by the Society, by corporate and other donors, and by the Division of Research Resources in the U.S. National Institutes of Health.. For additional information including how to contact the editor, see the box "About This Publication" on p. 23.

#### FELLOWS OF THE INTERNATIONAL EPR(ESR) SOCIETY

- ANATOLE ABRAGAM
- GEORGE FEHER
- . BREBIS BLEANEY
- RALPH HAHN
- CLYDE HUTCHISON
- . J. H. VAN DER WAALS
- ALEKSANDR PROKHOROV
   SAMUEL WEISSMAN

#### About Kev Salikhov:

From 1954-1959, Kev Minullinovich Salikhov, a native of Tatarstan, was a student of Prof. S. A. Altschuler in Physics at the Kazan State University. From 1959-1962, he was Aspirant of the Institute of High Molecular Compounds of the Academy of Sciences of USSR (Leningrad), his work there culminating in a Candidate of Sciences Thesis: "A Development of a Molecular Theory of Dielectric and Mechanical Properties of

> Polymer Glasses Concentrated Solutions." (1963) with supervisors Prof. M.V. Volkenstein and Prof. Yu. Ya. Gotlib. From 1963 to 1988 he rose through the ranks in the Institute of Chemical Kinetics Combustion of the Academy Sciences of USSR (Novosibirsk), becoming main researcher in 1986 and also serving on the faculty of Novosibirsk State University from 1967, becoming Professor in 1980. In 1974, he was awarded the Doctor of Sciences degree for his thesis "Kinetics of Processes Induced by Spin-Spin Interactions in Magnetically

Diluted Systems." He won the Lenin Prize in 1986 and in 1988 T aı R

ccepted the call to be Director of the Zavoisky Physical
echnical Institute of the Russian Academy of Sciences, Kazan
nd Professor at Kazan State University. In 1991 he was made
ull member of the Academy of Sciences of the Tatarstan
Republic; in 1992, made Vice-President of the Kazan
•
DIAMIO IOCHE

IN THIS ISSUE	
Salikhov Wins IES Gold Medal	1-2
Lebedev Succumbs	
From the Editor	2-3
Feher, McLauchlan Win Awards	3
International EPR(ESR) Society Affairs	
From the President (K. McLauchlan)	
The Computer Corner (K. Madden)	4-7
EPR Specialist Vignettes (A. Schweiger, ed.)	
The Linear Electric Field Effect in EPR (W.B. Mims)	
Building the Perfect Beast (C. Bender)	
Books and Proceedings	14-15
EPR Around the World (Azerbaijan - Aliev, Kerimov, Alieva)	
Notices of Meetings	
From EPR Centers (Center at Dartmouth)	21
Positions Available & Wanted	
Equipment & Supplies Exchange	23
Announcements (Mailing lists; Info. on WWW; E-mail updates).	23
About this Newsletter (The Masthead)	

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

Scientific Center of the Russian Academy of Sciences, in 1994 recognized as an Outstanding Scientist of Russia, and in 1996 named Honored Scientist of Russia and as Eminent Scientist of RIKEN (Japan). He has numerous other honors, serves on editorial boards, and is founder and Editor-in Chief of the international journal *Applied Magnetic Resonance*. He has been a member of the AMPÈRE committee since 1990, and was Fellow of Wissenschaftskolleg zu Berlin in 1992-3.

He has contributed essentially to the theory of phase relaxation induced by the spin-spin dipole-dipole interaction of paramagnetic centers in magnetically diluted solids; established exact limit behavior of electron spin echo envelope decay induced by the so-called spectral diffusion mechanism; found an analytical expression for electron spin echo envelope decay due to instantaneous spectral diffusion; theoretically demonstrated the possibility of electron spin echo envelope modulation caused by an anisotropic hyperfine interaction in disordered systems; for the first time demonstrated theoretically the role of selectivity of pulses in electron spin echo envelope modulation experiments; suggested an original approach to describing electron paramagnetic resonance experiments with nitroxide radicals undergoing ultra-slow rotational motion.

He has formulated new kinetic equations and using them, elaborated a theory of bimolecular Heisenberg spin exchange; for the first time calculated cross-sections of the following processes: spin exchange in solutions between free radicals and paramagnetic complexes, spin exchange between free radicals for a diffusional motion of particles in an interaction region, spin exchange between paramagnetic particles with an anisotropic distribution of the spin density, quenching of triplet positronium by paramagnetic complexes and free radicals. A new mechanism of the EPR line shift associated with the Heisenberg exchange interaction was theoretically predicted. He gave a theoretical interpretation of the first experimental observation of an external magnetic field effect on radical reactions in solutions; suggested kinetic equations to describe recombination of radicals in solutions which take into account the spin dynamics of radical pairs; developed the method of summation of contributions of all re-encounters of radical pairs on their recombination; predicted extrema in a field dependence of radical pair recombination probability and gave an interpretation of these extrema. He has obtained several interesting results concerning spin polarization in chemical reactions: theoretical prediction of the stimulated nuclear spin polarization effect in radical pairs recombination, analysis of regularities of CIDNP in low magnetic fields, a vector model of formation of chemically induced electron spin polarization (CIDEP), prediction of optical spin polarization induced by intersystem single-triplet transition in molecules in gas phase.

He has predicted quantum beats of EPR line intensities of radical pairs in photosynthetic reaction centers, formulated necessary conditions for creation of a spin coherence in the course of chemical reactions, suggested an algorithm for spatial design of spin polarization in solids.

Among Prof. Salikhov's current scientific concerns are the following projects: chemical reactions and coherence phenomena, particularly spin coherence; spin dynamics in a sequence of two radical pairs in a reaction center, contribution of hyperfine interaction to the spin dynamics in a reaction center; multiquantum effects in stimulated nuclear spin polarization for reaction in micelles; optically detected NMR of short-lived radical pairs; EPR study of a triplet of fullerenes and ion-radical pair states; optical studies of fullerenes; investigation by EPR imaging of the diffusion of spin labels into polymers; spatial design of spin polarization in solid paramagnets; study of nanostructures with scanning tunnelling microscopy and atomic force scanning microscopy; NMR imaging problems.

His hobbies: fishing, Tatar songs, being late to meetings. (Adapted from information sent by Prof. A. Il'yasov)

## LEBEDEV SUCCUMBS

As this issue goes to press, we have just learned the grievous news of the death of eminent EPR spectroscopist Professor Yakob Lebedev of the Institute of Chemical Physics of the Russian Academy of Sciences in Moscow. Professor Lebedev succumbed in Moscow after a brief illness. He was not only a world-class scientist but also our friend and colleague as well as a very active member and recent medalist of the IES. We all shall miss him very much!

## From the Editor—

"It was the best of times, it was the worst of times." So wrote Charles Dickens (A Tale of Two Cities, 1859), and so I feel now as the officers of our Society change. The past three years have been the best of times as I have had the privilege of working with outstanding scientists and the joy of interacting with such fine and decent human beings - Keith McLauchlan (President), Karl Hausser (Vice-President), Arthur Schweiger (Secretary), and David Greenslade (Treasurer) as well as Hal Swartz (Past President). They have worked hard to make the Society work well for all its members and given me a great deal of sound advice regarding the Newsletter as well as strong support and encouragement at just the right times. It is the

Publication of the International EPR(ESR) Society

worst of times because Keith, Karl, and David are leaving office and so, I fear, we will not be hearing from them so much. I have especially appreciated the enormous attention and energy that Keith McLauchlan has focused on the presidency of the Society and will miss the frequent, extensive, and thoughtful e-mail messages from him. (Keith, your good advice will be just as welcome after you've left office as before.) I sincerely hope that we have seen the worst of financial times for our Society and our Newsletter. We all have had to struggle to make this Society thrive financially and we cannot yet afford to do all the things for our Society and our profession that we would like to do. The officers have done wonders. However, it is up to not just the officers but to all members, individual and corporate, to see to it that the Society has better financial fortunes in the coming years. Finally, it is the best of times because the extremely energetic and perceptive Art Schweiger, who has contributed in a major way to making our work here in the Society and Newsletter offices both easier and better, has agreed to stay on as Secretary and because I look forward to some great ideas and hard work from the new officers - Jim Norris, Klaus Möbius, and "Raman" Kalayanaraman. Welcome!

I heartily congratulate Keith McLauchlan, Art Schweiger, Sandra and Gareth Eaton, and all the others who so beautifully planned, organized, and carried out the Society's Award events held this July on the occasion of the 19th International EPR Symposium in Denver. In each of its next few issues, the EPR Newsletter will feature one or more of the various honorees.

R. Linn Belford, Editor

## Feher Wins the Zavoisky Award; Bruker Award Goes to McLauchlan

Prof. George Feher of UC San Diego has been named the 1996 Zavoisky Award winner. Prof. Keith McLauchlan of Oxford Univ. has received the Bruker Award for 1997. Details for both awards will be included in a future issue of the EPR Newsletter.

**♦ IES AFFAIRS ♦**ANNOUNCEMENTS AND
REPORTS FROM THE INTERNATIONAL EPR SOCIETY

## The President's Valediction —

Three years ago you were kind enough to appoint me President of the IES, for which I shall always be grateful. The Office has proved both satisfying and enjoyable. These years have seen the Society attain truly international status, with 1400 members now in 57 different countries, and since their inception our awards and fellowships have gone to such distinguished scientists that our academic pedigree is established. At one stage I thought we made too many awards each year, but now I am all-too-aware of the many eminent people who still await recognition, and I am completely confident that the standards will be maintained. By any world measures we have a very successful Society in terms of membership and activity, although we all recognise further goals we should like to attain.

I have had the good fortune to be President when some of this has been accomplished, but whilst it is flattering to be suspected of being responsible for it, nothing could be further from the truth. I have been blessed with a wonderful Main Committee, and outstanding helpers. Hal Swartz established the basis for our present position when he was our first President, and has been a permanent source of advice and encouragement to me, besides always working hard to increase membership, improve relations etc. on his own. Karl Hausser has provided wise counsel of the very best sort as Vice-President. He has whispered in my ear when he thought advice was needed but has always encouraged me to act on my own judgement. Arthur Schweiger has been an exemplary Secretary in an Office whose function was not clear to either of us when he took over. He has established this, and has taken ever-increasing responsibility whilst at the same time acting as the conscience of the Society. To a good approximation all the really important personal touches which have been introduced and which have established a human face for the Society have emanated from him. David Greenslade worked hard as Treasurer before changed commitments caused him to have to demit office early. He has been replaced as Treasurer by Raman Kalyanaraman whose ability, energy and enthusiasm for the task and for the Society makes me feel positively old. The Regional Treasurers have laboured for the Society with little public recognition, but their work is both essential and greatly appreciated. Linn Belford has continued in his quiet and very professional way to edit and improve the Newsletter; his reliability and sureness of touch have been a Godsend. Becky Gallivan, assisted by Martha Moore, has taken responsibility for almost every aspect of the Society's affairs, a spectrum of matters which would astonish the reader to be told. No-one can ever have given more dependable or more able help and advice to any President anywhere; she would grace the White House (although the competition there might not be great!).

All of these wonderful people, whom I scarcely knew three years ago, are now personal friends to whom I shall always be in debt. They have worked unselfishly on your behalf without enjoying the public recognition of the President, and I offer them my sincere personal thanks.

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

So I leave Office with mixed feelings. I have enjoyed myself so much that it is sad to go, but the vitality of any Society needs new ideas to be introduced periodically, assumptions to be examined, and new goals to be identified. I write this as the election of my successor is underway, and I trust that the suggestion of the Main Committee of Jim Norris as President will be confirmed. If so, I could not leave the Office in safer, more considerate or more dynamic hands, and I look forward very much to helping him develop the Society in his turn. I have already had a session with him about the Society and, being Jim, he accepted at least half of what I said!

The IES is, and always will be, only as distinguished and important as its members. It is, quite simply, your (indeed our) Society, and ultimately it is you who I must thank for your help and support over the past three years. I do so with all my heart.

Keith McLauchlan

# Awards — All 1997 Nominations Due by Jan. 1, 1997

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 among the groups each year, with the three following loosely-interpreted categories: chemistry, physics and instrumentation, and biological sciences (including medicine). These categories are meant to be interpreted very liberally and not to be restrictive.

In 1997, three major awards, the IES Gold Medal, the Bruker Prize, and the Zavoisky Prize will be devoted to the recognition of outstanding achievements in EPR. Prof. Larry Berliner is the continuing Chair of the IES Gold Medal Award Committee.

Gold Medal: Nominations for the 1997 Gold Medal, recognizing benchmark contributions to EPR spectroscopy in Biology/Medicine, should be sent to Prof. Larry Berliner, Chairman of the Gold Medal Committee (e-mail: lberline@magnus.acs.ohio-state.edu) by January 1, 1997.

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, and Jan Stankowski. For Chemistry - Bruce Gilbert, Chair; N. Hirota, Jim Bolton, and Kev Salikhov. For

Biology/Medicine - Harold M. Swartz, Chair; Marjeta Sentjurc, Hideo Utsumi and 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. James R. Norris, Jr.

Fellows of the Society: The IES has created Fellowships to recognize truly outstanding contributions and achievements in electron paramagnetic/spin resonance among distinguished scientists (hopefully, IES members) who are either retired or are close to retirement. (Fellows of 1996: Erwin Hahn, J. H. van der Waals, George Feher). As the highest international standards are to be applied to the recognition of those worthy of this distinction, their formal connection with the Society will enhance its own image. Nominations for consideration by the Committee are to be sent in confidence by January 1, 1997 to Prof. James R. Norris, Jr., Univ. Chicago, Dept. Chemistry - Searle 133, 5735 S. Ellis Ave., Chicago, IL 60637 USA; 2: 1-312-702-7864; FAX: 1-312-702-0805; e-mail: j\_norris@uchicago.edu.

#### THE COMPUTER CORNER

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

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

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 (richard.cammack@kcl.ac.uk)
Dave Duling (duling@hippo.niehs.nih.gov)

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

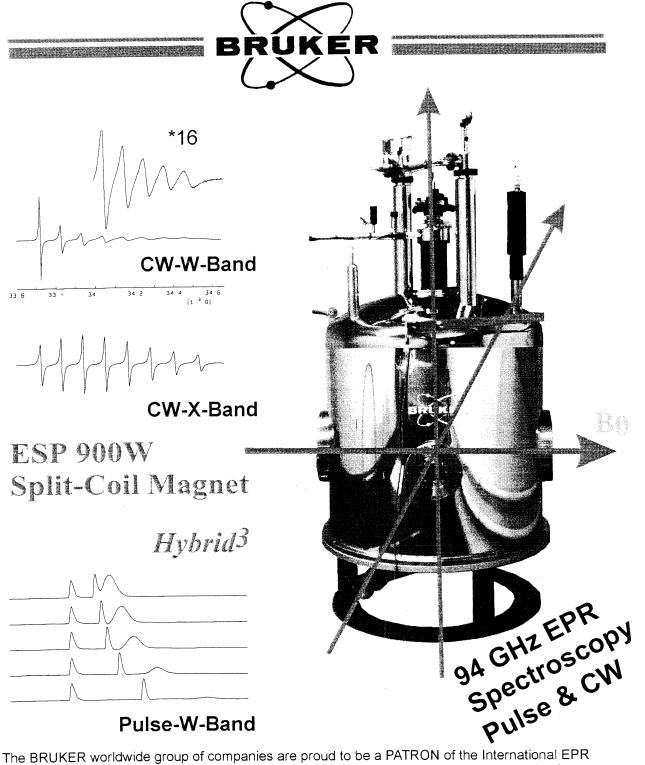
LINUX on a PC

by Keith P. Madden

University of Notre Dame, South Bend, ÍN, USA

In the last installment of our discussions on Linux, I presented the advantages of an open, free, and complete, supported operating system. In the next few installments of Computer Corner, I'll give you an overview on setting up Linux on your PC, with a view towards the issues involved in both trial and permanent installations. The information is valuable but it cannot be comprehensive in the column space available. Fortunately, complete information concerning Linux exists on the world wide web, at the home page of the Linux documentation project (http://sunsite.unc.edu/mdw/). This site contains links to the current edition of the Linux Frequently Asked Questions (FAQ) document, the Linux Information Sheet, and the numerous HOWTO documents giving full documentation

Publication of the International EPR(ESR) Society



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: 49-721-51 61-141; FAX: 49-721-51 61-237; email: epr\_sales@bruker.de. In the USA, contact Dr. Arthur Heiss, BRUKER Instruments, Inc., 19 Fortune Drive, Manning Park, Billerica, MA 01821. Telephone: 508-663-7406; FAX: 508-670-8851; email: ahh@bruker.com.

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

on the various technical details of Linux (file systems, networking, video configuration, etc.). It's the best place to seek information on Linux-related topics. I'll refer to this information at several points in this narrative.

#### Where to Get Linux

One important pre-installation question is that of where to obtain Linux. The Linux operating system, bundled with the necessary utilities, installation software, and selected applications, is called a distribution. There are quite a few of these available and are discussed in the Linux FAQ document. The most complete distributions are sizable collections of software, and are best acquired as a CD-ROM, although a less complete version of many distributions can be acquired by downloading from the FTP repository at sunsite (http://sunsite.unc.edu/); my first experience with Linux involved the Slackware distribution obtained this way (downloading ten floppy disks over a 14.4 kbs modem line). The distributions that I have used, roughly in increasing order of cost, are Slackware (packaged by Patrick Volkerding, available via ftp from Linux's sunsite, or on a CD-ROM from Morse Telecommunications, http://www.morse.net - no known relation to the editor of this column), Red Hat (Red Hat Commercial Linux, http://www.redhat.com), and the Desktop (Caldera, Network http://www.caldera.com). Slackware from sunsite is free via ftp (except for the time required to download it) and allows the user to select the utilities and applications to download. At this price level (free), your support will come from Internet Linux newsgroups. If you purchase a Slackware CD-ROM from Morse Telecommunications, you'll get a complete distribution, complete machine readable documentation, and installation support from the vendor. The Red Hat distribution on CD-ROM has many of the same good features, and includes their slick, proprietary installation program. Red Hat optionally bundles printed manuals with their distribution, for users who prefer hard copy. The Caldera distribution is the Red Hat distribution, augmented with licensed commercial components, including a Netware client from Novell, the Netscape web browser, and a "lite" version of the Crisp editor. Caldera bundles their distribution with their own printed

documentation, and provides support during and post-installation. Caldera sells office applications such as WordPerfect for Linux, and markets commercial add-ons for Linux, such as the WABI windows emulator pioneered by SunSoft. This array of distribution options means that you can select the expense and support level suitable for your budget and expertise. (Editor's note: watch which version of SlackWare Linux you are receiving. The current version is 3.1.0). There are many other good options not mentioned above - consult the web sites for further information.

#### Hardware Required for Linux

Linux is designed as a multi-tasking multi-user UN\*X workalike. To achieve the secure concurrent execution of multiple processes, Linux depends upon use of virtual 8086 mode by the CPU. This limits Linux usage to Intel or Intel-look-alike CPU-bearing PCS with 80386 or better processor. A multi-tasking environment also requires a large amount of memory to store the instructions and data for the multiple tasks in memory. A minimum of 8 MB will be quite usable for the Linux command line environment. The GUI environment, X windows, would be slow with 8 MB; with 16 MB of memory this subsystem works well. Since Linux is user-supported, its device-driver support comes from the group of users that have the particular board in their system. The result is that the ideal Linux system has a video, network, or I/O card that is the best performer in the (n-1)th generation of computer products, where n represents the current model. It takes a while to get drivers for the latest cards written and debugged. Suffice it to say that if you have a fairly fast, standard 486 or Pentium-based ISA bus machine containing 16 MB of RAM, using a IDE hard disk drive as your boot device, with a good, but not cutting-edge accelerated video card, you are highly likely to be successful installing and running Linux. The Linux Information Sheet supplies more details on compatible hardware, with the Linux Hardware Compatibility HOWTO providing the definitive listing.

A functional Linux installation will consume approximately 50-200 MB of hard drive space, depending upon one's restraint in installing optional applications, so you'll need at least this much space. Since this can be a trial

# Summit Technology Inc.

8827 Osceola Ave.

Morton Grove, IL 60053

Phone: 1 800 735 6327 / 847 470 1638

Fax: 847 470 1562

Email: 73173.1415@compuserve.com

http://ourworld.compuserve.com/homepages/summit1

## Supporter of the International EPR Society

- EPR Spectrometers
- Microwave Bridges
- Magnetic Field Controllers
- Variable Temperature Controllers
- Spectrometer Repair and Modification
- Visit our home page on the world wide web

Publication of the International EPR(ESR) Society

arrangement, prudence would dictate planning for the de-installation of Linux if it doesn't suit your needs. Speaking from experience, the best situation is to use a separate, spare hard drive for the Linux installation (perhaps one's old 250 MB drive that was recently replaced by a 1.6 GB monster), so that the entire Linux suite can be in on one separate hard disk in your computer. The reason for this implementation is that although PC-based Linux hard drives use the same low-level format as their DOS/windows counterparts, the higher level formatting details are different when using the Linux native file system EXT2. More recent CD-ROM Linux distributions, such as Slackware from Morse Telecommunications, allow one to run a live version of Linux off the CD-ROM, after booting the PC into Linux via a boot floppy disk copied off the CD-ROM. Since CD-ROM drives are slower than enhanced IDE hard drives, Linux runs appreciably more slowly than in a normal installation; this, however, is the minimally-invasive setup for trying Linux. Another relatively unobtrusive way to test Linux would be to install the Linux system using UMSDOS as the default file system. UMSDOS is compatible with DOS FAT partitions, so that the system files, application executables, and data can be installed on the pre-existing hard drive setup, with a boot floppy used to start Linux. These three methods allow us to test Linux without permanent commitment. We'll outline the UMSDOS installation in the next installment of this column.

\*\*\*\*\*\*

## EPR SPECIALIST VIGNETTES

Edited by Arthur Schweiger

### Electron Paramagnetic Resonance Imaging of Biological Samples

by Periannan Kuppusamy and Jay L. Zweier
Cellular and Molecular Biophysics Laboratories
Division of Cardiology, Department of Medicine
The Johns Hopkins Medical Institutions
5501 Hopkins Bayview Circle
Baltimore, Maryland 21224, USA

#### INTRODUCTION

After a decade of development and experimentation, the fields of electron paramagnetic resonance (EPR) spectroscopy and imaging (EPRI) have advanced to the point of enabling useful physiological and biochemical information to be obtained from living tissues (1-3). The development of low frequency EPR instrumentation at L-band, 1-2 GHz, or lower frequencies, and lumped circuit resonators has made it possible to perform EPR measurements on these lossy samples. Previous *in vivo* or *ex vivo* EPR spectroscopy studies have focused on global measurements of free radical metabolism and measurements of tissue oxygenation. Studies that require

## WILMAD GLASS Co.

# is a CONTRIBUTOR to the International EPR Society

"Serving the Spectroscopic Aftermarket"
EPR Glassware/Quartzware. Sample cells. Dewars.

Address:

Route 40 & Oak Rd.

Phone/FAX:

Buena, NJ 08310, USA 609-697-3000 / 609-697-0536

measurements of the spatial distribution of free radicals within the sample (EPR imaging) can be performed with magnetic field gradients in a manner similar to that of NMR imaging. EPR imaging, however, is faced with technical problems that make this technique more difficult to achieve in practice than that of NMR. The linewidths associated with EPR signals are 3 orders of magnitude larger compared to that of NMR signals and hence EPR imaging requires 100-1000 times more powerful gradients. Further, the paramagnetic centers to be studied are present in submillimolar concentrations compared to more than 100 molar concentrations of water protons utilized in NMR imaging. In addition, the EPR absorption function of most stable paramagnetic labels contains multiple lines due to hyperfine coupling. During the last few years significant progress has been made to enable the performance of EPR imaging of biological samples with improved image resolution and quality to obtain useful information. A brief overview of the technique and its application to biological systems is presented in the following sections.

#### **PRINCIPLE**

EPR imaging uses image reconstruction from projections. The goal of image reconstruction, in general, is to recover the spin distribution function f(s) from projections, where s is a coordinate in a given dimension. In three-dimensional (3D) spatial EPRI the recovered function is f(x,y,z), where x, y, and z are the Cartesian coordinates. Projections of the spin distribution (object) are obtained by performing a conventional EPR spectroscopic sweep in the presence of field gradients. It is assumed that the static magnetic field Bo, magnetic components of the microwave field and modulation field are homogeneous within the volume of the object. In the imaging experiment a gradient vector G of constant length is rotated along the surface of the sphere. During the field sweep, successive pseudo 'isofield' planes orthogonal to the gradient G are brought into resonance. The plane integrals of the EPR absorption function collected as a function of sweep field give a 'projection' of the object for the particular gradient or view. The planes are evenly spaced along the gradient vector according to the radial sampling interval. The G

# JEOL USA, Inc.

Manufacturer of CW Electron Spin Resonance Spectrometers Featuring a Compact Design with High Sensitivity and High Reliability

11 Dearborn Road, Peabody, MA 01960, USA Phone: 1-508-535-5900; FAX: 1-508-536-2205 E-mail: dipas@jeol.com

itself is angularly sampled in the polar coordinate system to give a series of projections. Image reconstructions are commonly performed by filtered-backprojection or Fourier reconstruction techniques. In addition, a variety of projection and image data processing techniques, including missing angle algorithm, spectral deconvolution, hyperfine correction are utilized to improve the quality and resolution of the reconstructed images.

#### SPATIAL AND SPECTRAL-SPATIAL IMAGING

EPRI can be performed in purely spatial space to obtain one, two- or three-dimensional (1D, 2D or 3D) images of free radical distribution. This usually requires 1 to 3 sets of gradient coils. 3D spatial imaging is necessary to obtain a

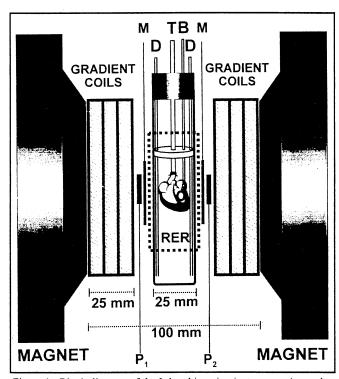


Figure 1. Block diagram of the L-band imaging instrumentation and rat heart placement. The tube containing the heart is placed in the central bore of a ceramic 3-loop-2-gap reentrant resonator (RER). Legends: M, modulation coils; P<sub>1</sub> Hall probe; P<sub>2</sub> Gaussmeter probe; T, perfusion tubing; D, drainage tubing; B, balloon tubing. The gradient coil assembly consists of three sets of water-cooled pair-coils for generating field gradients in 3D space.

complete unambiguous image of an asymmetric object. The 3D spatial reconstruction procedure assumes that the spectral shape is invariant throughout the object. Since the line shape information is totally disregarded in 3D spatial imaging, the information obtained is limited to only the spin content and not the nature of the line shape in the spatial volume element. To overcome this limitation Maltempo et al. (4) have developed spectral-spatial imaging wherein information is obtained over an additional spectral dimension (field axis) using multiple field gradients. This was followed by the development of 2D (1-spectral-1spatial), 3D (1-spectral-2-spatial) and 4D (1-spectral-3spatial) spectral-spatial imaging. The potential application of the spectral-spatial technique has been recognized in performing EPRI oximetry, based on the effect of oxygen in causing line broadening (5).

#### RESONATORS FOR EPR IMAGING

EPR imaging of biological samples has many technical challenges for instrumentation development in general, and for the sample resonator design in particular, beyond those of simple spectroscopy (see Figure 1). The most important is the need for a resonator design of minimum thickness, which makes it possible to achieve higher magnetic field gradients for a given coil's driving power. Thinner resonators also enable multidimensional gradient coils to be placed in the magnet gap. Loop-gap resonators (LGR) provide straightforward design and high filling factors. However, due to the open structure of the inductive loop element, LGRs require a shield. The need for the shield leads to problems in achieving an optimum magnitude of modulation field and a minimum 20 per cent increase of overall resonator thickness. Re-entrant resonators (RER) do not require a shield and can be constructed from ceramic materials to have high stability. A variety of low-frequency resonant cavities suitable for lossy biological samples have been developed, which enabled spectroscopic and imaging measurements on biological samples (6,7).

#### IMAGING OF BIOLOGICAL SAMPLES

Over the last decade, EPR imaging experiments have been performed by a number of groups around the world, on a variety of biological samples. While the aim of this article was not to give a review of these studies, we have used some typical examples from our own work to illustrate the application of the technique.

In our efforts to study the mechanism of free radical production and metabolism in biological organs such as the heart, we have developed instrumentation capable of performing spectral-spatial and spatial imaging. The imaging instrumentation consists of an L-band bridge, ceramic RER or surface coil resonators, three sets of water-cooled gradient coils with a Bruker signal channel and field controller interfaced to a personal computer. A Maxwell pair was used to generate the gradient along the z axis (the direction of the static magnetic field) and 2 sets of square pair coils were used to generate the x and y gradients. The

Publication of the International EPR(ESR) Society

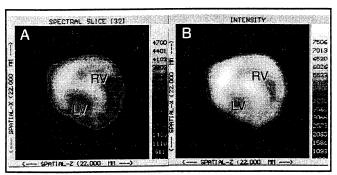


Figure 2. Cross-sectional transverse spatial EPR image (22 mm x 22 mm) of the rat heart perfused with 1 mM TEMPO obtained from a 3-D spectral-spatial image. A: Mid spectral slice B: Intensity map. The structure of the left ventricle (LV) and right ventricle (RV) are observed in the EPR image to be similar to that of a short axis histologic tissue slice. Projections 144; acquisition time, 16 min; spectral window, 8.0 G; maximum gradient, 27.4 Gauss/cm.

gradient assembly was capable of generating sustained field gradients of up to  $150~\mathrm{G/cm}$ .

The 3D spectral-spatial image of an isolated Langendorff perfused rat heart loaded with TEMPO is shown in Figure 2. The image corresponds well with cross sectional short axis sections through the rat heart as would have been expected from the orientation of the heart in the center of the resonator. A series of 3D spectral-spatial images were obtained as of function of global cardiac ischemia and used to obtain the spatial and temporal alterations in the metabolism of TEMPO and oxygen utilization (EPRI oximetry) in the heart during ischemia (7). Subsequently, we have also shown by computer simulations and by imaging phantoms and rat hearts that accurate 4D spectral-spatial images can be obtained that enable 3D mapping of oxygen (8).

Figure 3 shows a 3D spatial EPR image of an isolated ischemic heart infused with glucose char label. The glucose char material is highly oxygen sensitive with a linewidth of 0.19 G in the absence of oxygen and more than 100 G in

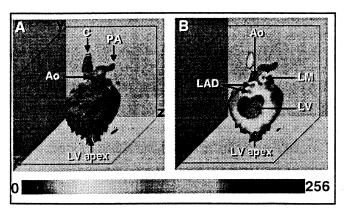


Figure 3. 3D images (25mm x25mmx25mm) of an ischemic rat heart infused with colloidal glucose char label. A, Full view of the heart; B, a longitudinal cutout showing the internal structure of the heart; Data acquisition parameters: projections, 1024; gradient, 50.0 G/cm; acquisition time, 78 min. Legends: C, cannula; Ao, aortic root; PA, pulmonary artery; LM, left main coronary artery; LAD, left anterior descending artery; LV, left ventricular cavity.

air. Thus, in air-equilibrated suspension or in the normally perfused oxygenated heart, no EPR image data can be obtained. However, under the severe hypoxic conditions that occur during ischemia this label can be used for EPR imaging. After 15 min of normal perfusion, the char label was infused and the heart subjected to no-flow global ischemia. EPR spectra were continuously measured to monitor the sharpening of the signal due to the decrease in oxygen concentration. The heart was then imaged by collecting 1024 projections. In the compiled 3D images shown in Figure 3, the external shape of the epicardium, large vessels including the aorta and pulmonary arteries, the internal endocardial surface of the left ventricle, the ascending aorta, aortic root, the left main coronary artery and the bifurcation of the left anterior descending coronary and the circumflex coronary arteries could be seen (9-10).

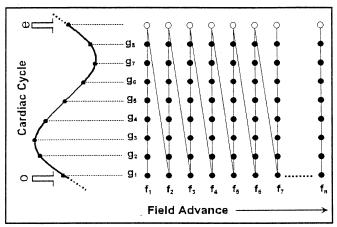


Figure 4. The principle of gated data acquisition. A sinusoidal wave is shown as the source signal for illustration. Data are collected at n field steps. At each step, the receipt of the pulse (odd pulse, o) triggers the acquisition of g number of data points (shown for g=8) over the cycle, data transferred, field incremented at e (even pulse, e), and acquisition continued at the receipt of the next pulse (o).

#### GATED EPR IMAGING OF BEATING HEART

Of the constraints that limit or compromise application of EPR imaging, the problems associated with organ movement, such as the contractile motion of the heart or respiratory motion with breathing, have considerably limited applications to living systems where motion occurs during the process of data acquisition. Thus, previous in vivo EPR spectroscopy and imaging studies had provided only time-averaged information. This results in a loss of information regarding the temporal and spatial changes. While random motional artifacts are difficult to control, periodic motions such as heart beat can be controlled by pacing at a fixed frequency and synchronizing the data acquisition system to that frequency, a process known as gated acquisition. Recently, we have developed instrumentation capable of performing gated imaging measurements on perfused beating rat hearts (11).

The principle of gated acquisition is schematically shown in Figure 4. The heart is paced continuously with a stimulator. The stimulator also outputs synchronized TTL

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

pulses that drive the data acquisition system. The gated data acquisitions are performed for each field step. When the field is set, the data acquisition will be triggered at the receipt of the next pulse and an array of g number of data points will be collected over the cardiac cycle by means of a high speed analog-to-digital converter. At the end of the cycle the field is incremented to the next step. The acquisition of the next cycle begins at the following pulse, and the process is repeated for a full sweep consisting of n discrete field steps. The resulting data array is then rearranged to give g number of spectra of n discrete samplings. The present instrumentation is capable of performing gated acquisitions of up to 256 images per cycle, with rates of up to 16 Hz. Thus a temporal resolution of 4096 Hz is possible at this maximum rate. We used 6 Hz  $(\tau=167 \text{ msec})$  pacing for perfused rat hearts and collected 16 points per cardiac cycle for 64 field steps. The typical data acquisition time was 25 sec per spectrum.

Gated EPR imaging measurements were performed on perfused beating hearts (11). The hearts were paced at 6 Hz. Gated projections were acquired with a field gradient of 20 G/cm. Vertical and transverse slices of 8 out of 16 images of the heart during a contractile cycle are shown in Figure 5. The contraction-relaxation cycle is clearly seen in these images. The systolic and end-diastolic pressures during the cycle were 120 mmHg and 8 mmHg, respectively. The aorta is identified at the top-left corner of the vertical slices in the figure. The LV cavity is clearly seen as the central void, and the two bright spots appear to correspond to the proximal coronary arteries. During systole, the LV cavity clearly narrows with vertical elongation. The LV wall also is seen to markedly thicken.

Recently we have also reported imaging of nitric oxide generation in the heart (12) and endogenous production of nitric oxide in the rat brain subjected to ischemia-hypoxia (13).

In summary, EPR imaging can provide unique information regarding free radical metabolism, tissue oxygenation, and nitric oxide formation, in a variety of important biological systems. While great progress has been made, further instrumentation development and optimization with extension to larger samples is needed to enable full realization of the great potential of this technology.

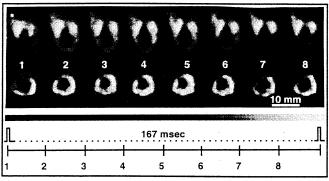


Figure 5. 3D spatial EPR images of the beating heart. A mid vertical slice (top row) and a transverse slice (bottom row) through the LV cavity are shown for 8 out of the 16 three-dimensional images of the perfused heart as a function of cardiac cycle.

#### REFERENCES

- L. J. Berliner, H. Fujii, H., X. Wan, and S. J. Lukiewicz, Magn. Reson. Med. 4, 380 (1987).
- H. J. Halpern, D. P. Spencer, J. V. Polen, M. K. Bowman, A. C. Nelson, E. M. Dowey, and E. A. Teicher, Rev. Sci. Instrum. 60, 1040 (1989).
- 3. G. R. Eaton, S. S. Eaton, and K. Ohno, (Eds.) "EPR Imaging and In Vivo EPR", CRC Press, Boca Raton, FL (1991).
- 4. M. M. Maltempo, S. S. Eaton, and G. R. Eaton, J. Magn. Reson., 72, 449 (1987).
- 5. R. K. Woods, J. W. Dobrucki, J. F. Glockner, P. D. Morse II, and H. M. Swartz, J. Magn. Reson. 85, 50 (1989).
- V. Quaresima, M. Alecci, M., Ferrari, and A. Sotgiu, Biochem. Biophys. Comm. 183, 829 (1992).
- P. Kuppusamy, M. Chzhan, K. Vij, M. Shteynbuk, E. Gianella,
   D. J. Lefer, and J. L. Zweier, Proc. Natl. Acad. Sci. USA 91, 3388 (1994).
- 8. P. Kuppusamy, M. Chzhan, A. Samouilov, P. Wang, and J. L. Zweier, J. Magn. Reson. B, 107, 116 (1995).
- P. Kuppusamy, M. Chzhan, and J. L. Zweier, J. Magn. Reson. B 106, 122 (1995).
- 10. P. Kuppusamy, P. Wang, and J. L. Zweier, Magn. Reson. Med., 34, 99 (1995).
- P. Kuppusamy, M. Chzhan, P. Wang, and J. L. Zweier, Magn. Reson. Med., 35, 323 (1996).
- 12. P. Kuppusamy, P. Wang, A. Samoilov, and J. L. Zweier, Magn. Reson. Med., 36, 212(1996).
- 13. P. Kuppusamy, S. T. Ohnishi, Y. Numagami, T. Ohnishi and J. L. Zweier. J. Cereb. Blood Flow and Metab. 15, 899 (1995).

## **GMW** Associates

- Laboratory Electromagnets & Power Supplies
- Precision Hall Effect Teslameters
- Digital NMR Teslameters
- Digital Voltage Integrators
- Precision Current Transducers

Specializing in Magnetic Measurements and Electromagnet Systems PO Box 2578, Redwood City, CA 94064 USA. Tel (415)802-8292 Fax (415) 802-8298

Publication of the International EPR(ESR) Society

## Building The Perfect Beast

by Chris Bender NIH Biotechnology Resource for Pulsed EPR bender@spin.aecom.yu.edu

### Tapered Waveguide and the Mims Cavity

For practical purposes, the Mims cavity can be regarded as a transmission mode bandpass filter. The resonator is a  $\lambda/2$  strip that bridges two parallel transmission lines. The two transmission lines are terminated in a short, and the resonant strip is located approximately  $\lambda/4$  from the short. The geometry and coupling mode dictates that the transmission lines (i.e. waveguide) tapers in the E-plane, and therefore a WR-90 guide decreases from a width of ~0.5" to 0.3". Although drawn symmetric in a figure that appears in a descriptive paper (ref. 1, Figure 3), the taper length/angle is asymmetric in the actual working unit. One section of waveguide tapers from a width of 0.5" to 0.3" over a nearly 1" distance whereas the other waveguide section achieves the taper in less than 0.5".

The Mims-style probeheads that I first used were built by John McCracken and were symmetric with respect to taper length and angle. I only discovered the asymmetry by accident when I started poking around our 'archives' and found a badly oxidized probehead of similar design. It turned out that it was Mims' original probehead 'rescued' from oblivion. Jim Anderson (Research Specialties) did a great job of cleaning and replating the piece, and I put it back into use on our spectrometer.

I rationalized the disparate tapers in terms of Slater's description<sup>2</sup> of tapered waveguide and simple mechanics. If you have a wave breaking on the shoreline, the 'violence' of the breaking wave (reflections etc.) is much less on a gently sloping shore than on an abrupt one. The more rigorous way to describe the tapers follows from wartime MIT Rad Lab work by Frank,<sup>3</sup> and expressed mathematically by Slater in his transmission line textbook.<sup>2</sup> The upshot is that the VSWR is higher on the steep transition than the gradual transition (the electrical engineer's way of describing a beach).

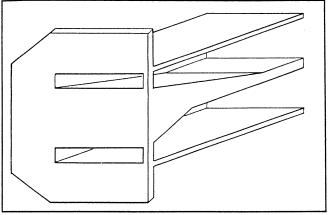
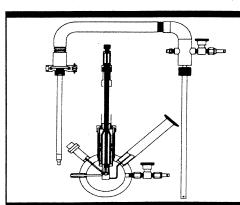


Figure 1: Cutaway drawing of the lower section of the Mims probehead, as electroformed for the Einstein lab (Mims apparently used an EDM process to manufacture the tapers, which are part of the flange). There are two parallel waveguide sections that end in (E-plane) tapers at the flange face; on the left is the gradual transmitter taper, and on the right is the steep receiver taper.

Now, on a pulsed EPR spectrometer there is a switch on the receiver's front end that protects the semiconductor components (mixer diodes and small signal amplifier) from the 25 W TWTA pulses. Although our spectrometer features an isolator on the receiver arm, I reasoned that Mims' intention was to provide additional attenuation (high VSWR) to the pulse power that is reflected by the closed receiver gate (ferrite isolators are typically directional to a degree of about 20 dB, and a fair amount of the 25 W pulse could therefore return). This would essentially keep the high power pulses going one way through the sample resonator, and thereby avoid spurious spin dynamics as a reflected wave/pulse returned to the cavity. Figure 2 is a simplified rendition of the geometry.

I gave a show-and-tell poster on the Mims design at last year's Denver meeting, and during the discussion someone suggested that the asymmetry was intended to distribute the echo energy preferentially towards the receiver. In other words, it was suggested to me that the short taper (looked at backwards) offers a higher impedance to the echo than the gradual taper. I had no data at the time to either argue pro or con to this interpretation of the design, but it gave me some food for thought, and I decided to look into the problem.



#### **EPR/ENDOR CRYOSTATS**

Complete Systems - Fastest Cooldown - Lowest Temperatures
Uses liquid helium or nitrogen - Push or Pull Operation
Plus, our replacement transfer line for your existing cryostat can Save you up to 50% on your liquid helium costs - Cool down samples faster
- Lower your terminal temperature and increase reliability!
Call or fax us for additional information:

**CRYO** Industries of America, Inc. 11 Industrial Way, Atkinson, NH 03811 Tel: (603) 893-2060; Fax: (603) 893-5278

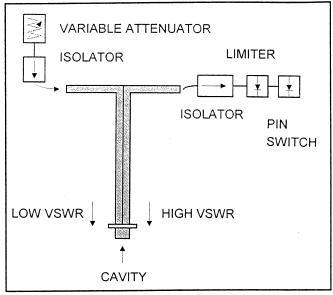


Figure 2: Simplified schematic drawing of the pulsed EPR spectrometer probehead and protection circuitry.

I can flip the probehead around and examine the echo amplitude directly, but I have to take into consideration the fact that, with the short taper now on the transmitter arm, the VSWR on the cavity input is presumably going to be higher. Any diminished echo amplitude would therefore be compensated by dropping the attenuation (our spectrometer features a Hewlett-Packard variable attenuator between TWTA and cavity) on the transmitter arm. As it turns out, I did not observe any difference in the optimized echo amplitude regardless of how I configured the probehead. I felt comfortable with this result, probably because of my bias towards a mechanical model. From the interior of the narrow section, I reason that a shock wave sees pretty much the same thing unless one wishes to claim that the 'roll off' is favored down the steep gradient. I imagine that the theory of horn antennas might be relevant to the problem of waves propagating into a waveguide section of an expanding taper, but there you are matching low to high impedance. Likewise, I did not find any relevant information in my household reference on shock wave propagation.5 I have made a mental note of setting up a ripple tank some day and experimenting with channels of differing depth.

The qualitative experiment of swapping the transmitter and receiver line during an experiment is not entirely convincing because, as I mentioned, I've altered the VSWR of the transmitter arm by reversing the probehead. I therefore decided to try an instructional experiment so that I would learn the nuances of waveguide plumbing. I made several 12" 'WR-90' sections of waveguide that ended in a taper down to interior dimensions of 0.9" x 0.3". These E-plane tapers approximate the dimensions of the Mims probehead. What I then wanted to do was launch a signal at a point between two dissimilar taper sections and use a vector voltmeter to compare the power

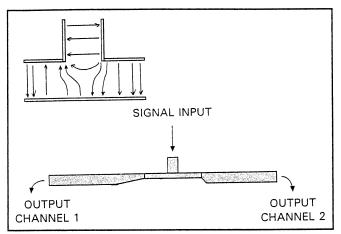


Figure 3: Tee circuit that was used with a vector voltmeter to test the power distribution between two tapered waveguide sections that are intended to simulate the Mims probehead. In the upper right corner a cross sectional view of an open junction Tee is illustrated with its E-field lines; the actual Tee used in this test was narrowed in the E-plane, as indicated in the shaded drawing.

distribution at the end of each arm. The 'launch' section was constructed from a modified waveguide open Tee-junction in the E-plane whose input was the standard WR-90 dimensions, and whose output arms were the same 0.9" x 0.3" dimension of the tapers. Figure 3 illustrates the apparatus.

Figure 4 illustrates a direct oscillographic trace of the waveform detected at the two arms of the Tee. The top trace corresponds to the arm bearing a 0.5" taper, and the bottom trace corresponds to a 2.0" taper. There is a slight variation with frequency in the relative magnitude of the waveforms, but this was found to be traceable to the coaxwaveguide transitions (reversing the channels reversed the

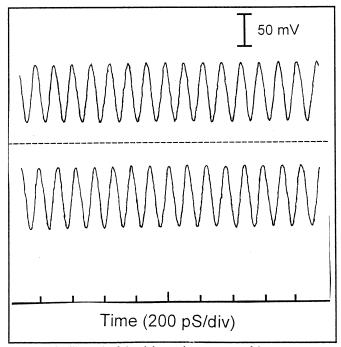
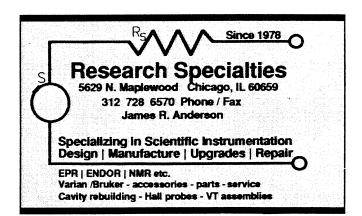


Figure 4: Oscillograph of signal detected at two arms of the apparatus illustrated in Figure 3. There is no significant difference between them.

Publication of the International EPR(ESR) Society



results). This result is verified quantitatively by using a vector voltmeter, which indicates that across the X-band frequency range (8 - 12 GHz), the two waveguide arms differ by no more than 1.6 dB (this amounts to a 30 - 40% discrepancy; the value is frequency dependent, and the dominant 'arm' likewise varies; typical variance between the two arms is 0.5 dB). These data therefore demonstrate that the waveguide tapers do nothing to add directionality to the echo power distribution.

I tested my original interpretation of the tapered waveguide reconfiguring the analyzer for scalar network measurements. After calibration I connected the entire probehead (tapered lines plus cavity) to the analyzer, and measured the scalar network parameters with the probehead oriented in both possible ways (i.e. steep or gradual taper on transmitter side). Figure 5 illustrates the results. With the probehead inserted so that the gradual taper faces the transmitter, the transmission profile resembles a low Q filter, as expected (Figure 5, top trace). In the reverse configuration (steep taper on the transmitter side), the probehead transmits virtually no power at any frequency (Figure 5, bottom trace). Surprisingly, however, if I perform the same experiment with the taper sections that I used in the Tee experiments (remove tee junction in Figure 3, and substitute the abutted tapers for the Mims probehead), I saw no significant difference in the transmitted power regardless of which direction the steep taper

Despite the results of this test, I still feel a bit ill at ease with these waveguide tapers, particularly in the pulsed spectrometer system. What bothers me is that wave transmission differs somewhat from pulse propagation<sup>4</sup> and there are various scattering effects that can occur when a shock wave strikes an obstruction such as a wedge (angle-dependent).<sup>5</sup> Most of these 'artifacts' of the EM field will be transparent to a Mims-type echo modulation experiment (much of the Mims experiment is intentionally designed to obviate artifacts of EM effects beyond the experimenter's control), but I sometimes wonder if these EM phenomena could modulate a spin system in such a way that would corrupt the data recorded in a spin coherence experiment. Just as an example, I think that for many of the phenomena described by Salikhov of the Zavoisky Institute, I would forgo resonant structures in favor of loaded transmission

lines, as used formerly by microwave spectroscopists. This would reduce the distortion of the propagating excitation pulse (one reduces the EM field problem to simply a propagation through dielectric medium rather than introduce the complexity of the lumped circuit of the resonator), which in the theoretical discussions is often assumed to be ideal in shape and lacking in sidebands. Towards an understanding of the pulse propagation I have been making large-scale versions (C- and S-band) of the Mims cavity and other resonators so that I might be able to insert probes with minimal perturbation and have more precise control over the cavity's geometry. I hope to get these things onto a pulsed microwave analyzer and fully characterize their behavior and response to high power pulses.

#### REFERENCES & NOTES

- 1. Davis, J.L.; Mims, W.B., 1978, Rev. Sci. Instrum., 49, 1095-7.
- 2. Slater, J.C., 1942, Microwave Transmission, McGraw-Hill, New York.
- 3. Frank, N.H., 1943, Tapered Transmission Lines and Wave Guides, Radiation Laboratory Report 189. Summarized in Ragan, G.L., 1964, Microwave Transmission Circuits (MIT Rad Lab Series Vol 19), Boston Technical, Lexington.
- 4. There is an excellent text on transmission line theory that includes an analysis of pulsed signals by Grivet, P., 1970, The Physics of Transmission Lines at High and Very High Frequencies (in two volumes), Academic Press, London. The English edition is out of print, but the original French edition is still available as Physique des lignes de haute fréquence.

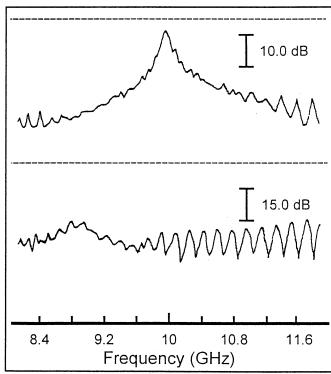


Figure 5: Scalar network (transmission) trace of Mims probehead. The top trace is recorded with the microwave source located on the side of the gradual taper, and the bottom corresponds to the measurement repeated with the source on the steep taper side.

5. Ben-dor, G., 1992, Shock Wave Reflection Phenomena, Springer-Verlag, New York.

**ACKNOWLEDGMENT** - Thanks to the Hewlett-Packard Corporation for their loan of a 71500 Transition Analyzer that was used in this study.

### Electromagnetic Field Probes

I recently had the opportunity to visit Clemson University's Microwave Measurement Laboratory. While taking a morning tour with one of its principal scientists, Chalmers Butler, I engaged in 'microwave-guy' talk about probes and field measurements (they run a course on field measurements as part of the electrical engineering dept curriculum). I learned a nifty little nugget of info about using inductance loop probes.

Normally, we fashion these probes out of coax by cutting away the outer conductor to expose the inner conductor, which is then bent to form the loop. The difficulty that they have, however, is that the exposed loop probe actually detects two field related items, namely the H-field (what you want) and the derivative of the E-field (what you may or may not want). To get around this unwanted (dE/dx) component they have devised a probe that uses a smaller diameter semi-rigid coax line as the loop. The loop is formed from the unmodified coax cable from which a small section of outer conductor is removed.

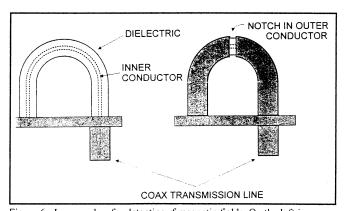


Figure 6: Loop probes for detecting rf magnetic fields. On the left is an unshielded loop (dielectric intact), and on the right is the modified (partially shielded) loop. The unshielded loop measures dE/dx (where x is the loop diameter, which may not be significant enough to warrant the tedium of making the notch). In the actual probe, the shielded section (loop) is microcoax, not standard 0.085 or 0.141 semirigid coax.

Figure 6 illustrates the familiar and modified probes.

Note: Finally, David Greenslade of Essex recently sent me a note that included a constructive remark regarding this column. The vendors that I specify are quite often US-based, and this poses problems for non-US groups. I would therefore welcome 'vendor reviews' on a country-by-country basis or, alternatively, volunteer editors to whom I could send pre-publication drafts of each column and get non-US sources of relevant supplies. Once again, my e-mail address is bender@spin.aecom.yu.edu.

## **BOOKS & PROCEEDINGS**

Reprinted copies of *SPIN LABELING: THEORY AND APPLICATIONS* (Lawrence J. Berliner, Ed.), Volumes I and II. to become available.

While Prof. Berliner still gets quite a few inquiries per year about how to obtain the first two volumes, he recently learned that Academic Press declared them out of print in summer, 1995. No more copies exist (at least to his knowledge). Amazingly, these volumes are still quite useful. Volume I is somewhat of a classic and has become a 'textbook'.

Prof. Berliner is arranging for Academic Press to grant a release of the copyrights and rights to reproduce them. If enough people express interest, the Illinois EPR Research Center, as part of its service to the EPR community, will run off an initial batch of copies with a binding and ship them to you. Details are still being investigated, but we know already that the cost to you would be a great deal lower than the publisher's most recent prices.

At this juncture, we need to find out how many people are seriously interested. Please e-mail or FAX Becky Gallivan at the IERC (ierc@uiuc.edu or 217-333-8868; full address in masthead at the end of this Newsletter). We would then respond to you with details of exact cost and the estimated run/shipping date. Please state your interest in Vol. I, II or both: SPIN LABELING: THEORY AND APPLICATIONS (Vol I), Academic Press (1976), 592 pages. Spin Labeling: Theory and Applications (Vol I), Academic Press (1979), 354 pages.

Larry Berliner, Linn Belford, Bob Clarkson

BOUNDARY ELEMENTS XVIII. Edited by C.A. Brebbia, J.B. Martins, M.H. Aliabadi and N. Haie. This book contains the proceedings of the 18th International Conference on Fluid Mechanics held at Braga, Portugal September 24-26, 1996. Thirteen sections cover these topics: Acoustics, Thermal Problems, Inverse Analysis, Electromagnetics, Numerical and Computational Aspects, Optimization, Stress Analysis, Fracture Mechanics, Geomechanics, Plate Bending, Fluid Mechanics, Flow in Porous Media and Wage Propagation.

Price: £199.00/\$299.00; ISBN: 1853124044. Available September 1996, from Computational Mechanics Publications, Ashurst Lodge, Ashurst, Southampton, UK S040 7AA; **\***: 44-1703-293223; FAX: 44-1703-292853; E-mail: cmp@cmp.co.uk.

2-MM WAVE BAND EPR SPECTROSCOPY OF CONDENSED SYSTEMS by Victor I. Krinichnyi. This is the first book summarizing the problems of utilization of modern high-resolution 2-mm wave band EPR spectroscopy in an interdisciplinary field for the investigation of various condensed systems. The

Publication of the International EPR(ESR) Society

### SCIENTIFIC SOFTWARE SERVICES

P.O. Box 406

Normal, IL 61761-0406 USA Voice/Fax: 309-829-9257

Contributor to the International EPR Society

Cost-effective EPR data acquisition, simulation, deconvolution, and imaging software for ALL EPR spectrometers.

Free DEMOs available.

CALL for further information and pricing

Web site: http://www.wwnet.com/~sss/

possibilities of obtaining additional information on molecular and electron processes in such complete solid-state objects, as enzymes, biological and organic conducting polymers are considered. This book is written for spectroscopists familiar with the basic principles of EPR and for physicists, biophysicists and chemists interested in new applications of the method. It can be used both as a textbook and a reference by graduate students in physics, biology or chemistry. The material is illustrated quite enough and is kept as diverse as possible. It is moderately theoretical, and manifold experimental aspects are discussed. The main subjects treated in the book include: Peculiarities of 2-mm EPR spectroscopy and appropriate experimental techniques; Dynamics and polarity of radical microenvironment in model and biological systems; Nature and dynamics of charge carriers and charge transfer mechanisms in organic polymer semiconductors; 2-mm EPR spectroscopy of low-dimensional ion-radical salts and high-temperature superconductors. For more information please contact: CRC Press, 2000 Corporate Blvd., NW, Boca Raton, Fl 33431, USA; **2**: 1-407-994-0555; FAX: 1-407-241-7856; E-mail: marketing@crcpress.com.

John Weil and Jim Bolton have established a WWW folder containing an up-to-date set of corrigenda for their textbook *ELECTRON PARAMAGNETIC RESONANCE* (Wiley 1994, reprinted 1995). A short description of the book's contents also is included. Access is available via:

http://chm15127.usask.ca. If you do not have access to the web, contact Prof. John A. Weil, Dept. Chemistry, Univ. Saskatchewan, Saskatoon, SK S7N 5C9, Canada; 2: 1-306-966-4658; FAX: 1-306-966-4730;

E-mail: John.Weil@usask.ca

## REPORTS ON EPR AROUND THE WORLD

## EPR IN AZERBAIJAN

by D. I. Aliev, M. K. Kerimov,\* and I. N. Alieva
Dept. of Physics, Baku State University, Azerbaijan
\*Sector on Radiation Investigations
Academy Sciences of Azerbaijan

The first EPR studies by Azerbaijanian scientists date to the mid-1960's, when EPR was just ceasing to be exotic. EPR in selenium was discovered and studied at the Institute of Physics of ASA (Academy Sciences of Azerbaijan)<sup>1-3</sup>, but no signal was found in amorphous powdery selenium of different purity. The almost symmetrical singlet without superfine structure with a g-factor of  $2.0035\pm0.0050$ , and line width  $\Delta H_m$ =5.5±0.5G appeared in selenium preparations exposed to oxygen and iodine after thermal treatment. The EPR signal intensity increased according to the Curie's Law over the range -196 to  $17^{\circ}$ C, g-factor and  $\Delta H_m$  remaining unchanged. Based on these temperature and relaxation effects, donor-acceptor charge transfer complexes were inferred to be the origin of this paramagnetism.

At the Institute of Inorganic and Physical Chemistry of ASA, EPR of metal ion complexes containing radical moieties was studied. In complexes with both Cu(II) and nitroxide, electron exchange interaction between the spin centers caused averaging of both g-factor and superfine structures of metal ion and radical.<sup>4</sup> In Co(III) and Pd(I) complexes containing phenoxyl radicals, electron transmission from electron donor fragment (sterically hard phenol) on the metal ion was established. Chelates having electron-donor fragments able to form stable single-electron oxidizing stages (cation radicals)<sup>5</sup> were studied.

### **ELECTRON SPIN RESONANCE VOLUME 14**

#### NEW VOLUME \* NEW APPROACH

From Volume 14 this series takes a fresh approach to its coverage of the literature in this important area. Its treatment is selective, critical and eminently readable, giving readers an authoritative insight into current trends and developments, in the key areas where ESR is being applied.

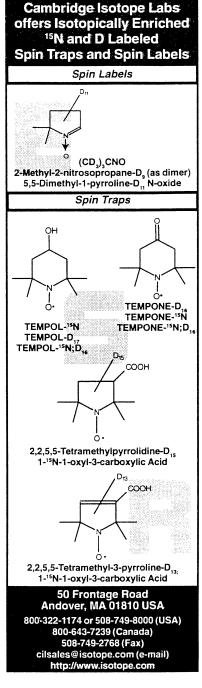
#### For further details please contact:

The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF, UK. FAX: 44-223-423429

#### Or in the USA, Mexico and Canada:

CRC Press, Inc., 2000 Corporate Boulevard NW, Boca Raton, FL 33532, USA. **\***: 1-407-994-0555.





Over the past few years, numbers of paramagnetic species in different catalytic systems have been identified, leading to better understanding the reactions catalyzed bу paramagnetic species. The possibility of a radical chain mechanism of catalytic degradation of poly(isobutylene) under the action of AlBr, and AlEtCl, in aliphatic solvents was considered.6 The role of single electron centers was discussed in the conversion of methane dimerization aromatization products.7 The nature and reactions paramagnetic species were discussed for polyoxometallates that photocatalyze hydrogen generation from water-organic solutions.8

One of the developmental directions of EPR spectroscopy in Azerbaijan was connected with studies of electric field effects polymeric dielectrics. The nature and mechanism of

formation and accumulation of free radicals in polymeric dielectrics under the influence of strong electric fields were established in the Sector on Radiation Investigations of the ASA. The effect of suppression of macroradical photogeneration in polymers under the influence of strong electric fields was discovered with the aid of spin-label methods. 10 EPR signals from surface-stabilizing electrons arising in the polymeric films in the coronal charge were discovered and studied.11

EPR studies of the kinetic mechanism of decomposition

of water molecules on the surface of oxide catalysts irradiated with X-rays defined the nature of radiationinduced paramagnetic centers and radiation-heterogenic processes involving MeO+H<sub>2</sub>O <sup>12</sup> systems.

At the Baku State University, it was established that in the presence of silicon molybdate - the specific acceptor of photosystem-2 (PS2) electrons into PS2 preparations - in the light, the dark-adapted signal appeared. The electronic relaxation characteristics and photochemical reactions of the paramagnetic center responsible for its EPR signal and belonging to the PS2 were proved. This EPR signal's parameters - g  $\sim 2.0025$ ;  $\Delta H = 9G$  - indicate that it arises from the cation radicals of monomeric chlorophyll. 13,14

At the Institute of Molecular Biology and Biotechnology of the ASA, EPR and spin-label studies of darkening and photoinduced free radical centers as well as the photoinduced structural changes of pigmentary epithelium and its melanoprotein granules in animal eyes and synthetic melanin were carried out and kinetic parameters obtained. It was established that visible light in pigmentary epithelium causes conformational changes at all depths of

## 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

the membrane, induced by the melanin.<sup>15</sup> In the model systems protein+melanin, lipid+melanin the antioxidant properties of synthetic melanin were studied. Melanin was shown to reduce the accumulation of paramagnetic centers in y-radiated albumin.16 The essential increase of free radical centers in pigmentary epithelium of eyes under acute hypoxia indicated a possible role of the melanin in regulating free radical processes in this tissue.<sup>17</sup>

Spin-label studies showed that the changes of thylakoid membranes induced by chemical substances correlate with changes of functional activities of chloroplasts of higher plants. 18 The mechanism of the influence of antioxidants propil-gallae and phenozane - on thylakoid membrane of chloroplasts was established. The free radical content of natural silk was shown to be defined by the numbers of microscraps in it. A correlation between the free radical concentration in natural silk and their physico-mechanical and technological characteristics 19 was established.

Scientists of the Institute of Physics of the Academy Sciences of Azerbaijan studied by EPR the free radical

Publication of the International EPR(ESR) Society

processes attending mechanical destruction of proteins.  $^{20,21}$  It was established that breaking the  $C_{\alpha}$ -C bond of the main peptide chain to form the radicals -NH-CHR and CO-NH-is the primary free radical act in mechanical destruction of proteins. The dynamics of changes of crystallic fibrillar proteins affected by the mechanodestruction were studied. The many stages of transformation of free radicals in the photo- and thermo-reactions in the mechanically degraded proteins were established.

In collective investigations by the scientists of the Baku State University, the Institute of Chemical Physics of the Academy Sciences of Russia, and the Sector on Radiation Investigations of the ASA, the interrelation of weakly bound non-heme iron (free iron) and nitrogen oxide (NO) incorporated with thiol groups of proteins into low-spin (S=1/2) paramagnetic complexes were studied in tissues of animals and plants 22,23 These complexes were characterized by a g<sub>av</sub>~2.03 EPR signal, so they are termed "2.03 complexes". It was established that in the bioobjects there were no endogenous ligands separate from the thiol and capable of forming complexes with free iron and NO. The 2.03 complexes were the only form of non-heme iron and nitrogen oxide coexisting in the biosystems. The free iron contained in leaves and fruits of higher plants can be detected by EPR during its incorporation into di- and mononitrosyl complexes with various anion ligands. On the basis of EPR together with quantum chemistry and theoretical conformational analysis, a structure of the 2.03 complexes with iron, two molecules of NO, two thiol ligands, and two molecules of solvent that can act to stabilize the structure was proposed.<sup>24</sup> Then the possibility of participation of 2.03 complexes as the other nitro- and nitrozo-containing compounds of endogenous and exogenous origin in NO metabolism in organisms was studied.

#### REFERENCES (\* denotes "in Russian")

- Abdullaev G.B., Ibragimov N.I., Mamedov Sh.V., Djuvarli T.Ch., Aliev G.M.; Dokl. Akad. Nauk Azerbaijan SSR, 20 (1964) 13.\*
- 2. Abdullaev G.B. et al; Phys. Stat. Sol., 16 (1966) k113.
- Ibragimov N.I., Aliev G.M., Abdinov D.Sh., Mektieva S.I., Mamedov Sh.V.; Uspechi fizisheski Nauk 2 (1969) 503.\*
- Medjidov A.A., Timakov A.A., Mamedova Y.G.; J. Strukt. Khim. 18 (1977) No. 4, 714.\*
- 5. Medjidov A.A., Kasumov V.T., Golubeva I.A., Rzaev R.Z.;

## RESONANCE INSTRUMENTS, INC. is a CONTRIBUTOR to

The International EPR Society

EPR spectrometers, components, accessories; Model 8320 Magnet Field Controller for Varian's Mark I & II, others, provides keyboard or computer control; microwave instrumentation to 170 GHz.

Resonance Instruments, Incorporated
9045 Terminal Drive, Box 1488, Skokie, IL 60077, USA
\$\pi\$: 1-847-583-1000 FAX: 1-847-583-1021

Koord. Khim. 17 (1991) no. 12, 1698.

- 6. Ismailov Et.G.; Acta Polymerica 91 (1990) 226.
- 7. Ismailov Et.G.; React. Kinet. Catal. Lett. 44 (1991) 19.
- 8. Ismailov Et.G.; Chemistry of High Energies 21 (1987) 356.\*
- 9. Gezalov Kh.B., Kerimov M.K.; J.Tek. Fiz. 52 (1982) 1386.
- Kerimov M.K., Tikhova Y.I., Gezalov Kh.B.; Khim. Fiz. 17 (1984) 1208.
- 11. Kerimov M.K.; Phys.Stat.Sol. <u>90</u> (1985) k71.
- Garibov A.A., Gezalov Kh.B., Kasimov R.D., Agaev T.N.;
   J. Radiat. Phys. Chem. <u>30</u> (1987) 197.
- Goldfeld M.G., Khalilov R.I., Khangulov S.V.; Molek. Biologiya 13 324.\*
- Khalilov R.I., Chomutov G.V., Tichonov A.I.; Physiologiya Rastenii 40 (1993) 339.
- Abdullaev G.B., Kerimaov T.M., Mamedov Sh.V., Yusifov E.Y.; Dokl. Akad. Nauk SSSR U254U (1980) 231.
- 16. Yusifov E.Y., Donzov A.E., Ostrovski E.Y.; Radiobiologiya 27 (1987) 8.\*
- 17. Magomedov N.M., Djavadov A.I., Yusifov E.Y.; Biofiz. 35. (1990) 977.\*
- Kerimov T.M., Bayramov Kh., Tichonov A.N.; Biofiz. 36 (1991) 128.
- 19. Kerimov T.M.; SHELK 3 (1984) 29.\*
- 20. Gasymov O.K., L'vov K.M.; Biofizika 33 (1988) 46.\*
- 21. Gasymov O.K., Mamedov Sh.V., L'vov K.M.; Polymer Sci. USSR Review Art. 34 (1992) 196.
- 22. Vanin A.F., Aliev D.I.; Studia Biophys. 93 (1983) 63.
- 23. Aliev D.I., Kurbanov I.S., Vanin A.F.; Studia Biophys. 115 (1986) 173.
- 24. (a) Aliev D.I., Alieva I.N., Godjaev N.M.; J. Fiz. Khim. <u>68</u> (1989) 2656; (b) Studia Biophysica <u>139</u> (1991) 17.

# NIKKISO Co., Ltd. SUMITOMO SPECIAL METALS Co., Ltd. SUPPORTER of the International EPR Society

Innovative Portable EPR Spectrometer with a built-in 32 bit computer (ES-10)

Frequency: 9.4 GHz

Sensitivity: 2\*1010 spins/0.1 mT

Resolution: 6\*10<sup>-5</sup>

Size: 500x500x230 mm

Weight: 25 kg

Magnet: NEOMAX-40



SUMITOMO SPECIAL METALS AMERICA, Inc. (Tel)310-378-7886, (Fax)310-378-0108

## **NOTICES OF MEETINGS**

#### OXYGEN '96, Eden Roc Resort & Spa, Miami Beach, Florida, USA, November 21-25, 1996.

Special events include the "Biological ESR Workshop" on November 21, and a "Sunrise Free Radical School" each morning. For information, contact Oxygen '96 c/o The Oxygen Society, 74 New Montgomery, Suite 230, San Francisco, CA 94105-3411, USA. : 1-415-546-3124. Lectures by Garry R. Buettner, Art Heiss, Colin F. Chignell, Ronald P. Mason, Walee Chamulitrat, B. Kalayanaraman, Ralph Weber, Harold M. Swartz, Jay L. Zweier. For more information about this workshop, including news about lecture topics, call The Oxygen Society; : 1-415-546-3124.

# 1st ASIA-PACIFIC EPR/ESR SYMPOSIUM, January 20-24, 1997, Hong Kong.

The aim of this symposium is to bring state-of-the-art knowledge of EPR and related magnetic resonance techniques to Hong Kong and southern China. The Symposium will constitute an unique opportunity to bring together active researchers, leading world experts, and potential users of EPR techniques. The Symposium, although aimed primarily at Asia-Pacific countries, is open to participants from all over the world.

In order to promote and facilitate collaboration among EPR/ESR researchers and users from the Asia-Pacific region, during the Symposium a special session for the Inaugural Meeting of the Asia-Pacific EPR/ESR Society (APES) will be held. The establishment of the Regional EPR/ESR Society, to be affiliated with the International EPR(ESR) Society, has full support of the parent Society. Areas of interest include: \*mineralogy including gemmology \*polymers \*EPR dosimetry and dating \*environmental science and protection \*fossil fuels \*medical applications \*biological and photosynthetic systems \*semiconductors \*magnetic materials \*high temperature superconductors \*ferroelectrics and optoelectronic materials \*new developments in EPR and related techniques.

Contributions will be in the category of either invited papers for plenary sessions or of contributed papers for either parallel topical sessions or poster sessions. Time for

## AMERICAN INSTITUTE OFPHYSICS

## **Professional Societies & Publications**

500 Sunnyside Boulevard Woodbury, NY 11797-2999 USA Phone: 1-516-576-2411 Fax: 1-516-576-2481

presentations at the plenary and topical sessions includes discussion. The Symposium language will be English. Four parallel topical sessions encompassing the following fields are planned: \*biology, life and medical sciences, \*chemistry, earth and environmental sciences, \*physics and materials science \*new developments and cross-disciplinary areas.

Abstracts of contributed papers will be refereed by the Scientific Programme Subcommittee with the help of external reviewers if necessary. A book of abstracts will be distributed to participants at registration.

For further information, contact the Symposium Secretariat, Dr. S.K. Wong, (\*s. 852-2788-7662; e-mail: apskwong@cityu.edu.hk) or Prof. Czeslaw Rudowicz, Chairman, Dept. of Physics and Materials Science, City Univ. of Hong Kong, 83 Tat Chee Ave., Kowloon, Hong Kong (\*s. 852-2788-787; FAX: 852-2788-7830; e-mail: apsepr@cityu.edu.hk). Information on the Symposium can also be found on the WWW home page: http://www.CityU.edu.hk/AP.

30th ANNUAL INTERNATIONAL MEETING: "ESR SPECTROSCOPY OF RADICALS IN ORGANIC AND BIOLOGICAL SYSTEMS" in conjunction with the 5TH INTERNATIONAL SYMPOSIUM ON SPIN TRAPPING: "APPLICATIONS IN CHEMISTRY, BIOLOGY AND MEDICINE", April 6-10, 1997, Lancaster, UK.

The 30th meeting of the ESR Group of the Royal Society of Chemistry, London will celebrate 29 consecutive years of International meetings on the topic of Electron Spin Resonance Spectroscopy. The meeting will be held at The Univ. of Lancaster, in conjunction with the 5th International

## **CPI Sets the Standard for EPR Klystrons**

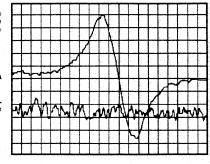
CPI Replacement Klystrons deliver:

- Optimum application flexibility Long Life
- Reliable performance, low noise New warranty
- X band for Century Series, E lines, plus Q band
   Now available directly from CPI. For more information call
   CPI at 1-800-843-8780 or 415-846-3188 from outside the U.S.



formerly a division of Varian®

taken with a Varian weak pitch sample in a TE182 cavity under the conditions specified in the Varian E Line Series unwordfied (E182E189 bridge) instruction menual. 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 .863 seutiplication factor. Without the suttiplication factor, the signal to noise would be 388:1.



Publication of the International EPR(ESR) Society

Meeting on Spin Trapping. The Conference opens with a reception and dinner on Sunday evening and closes after lunch on Thursday. The organisers extend a cordial invitation to all persons interested in ESR spectroscopy in Chemistry and Biology to attend. Accommodation will be in individual rooms in a residence hall on the campus, where the lectures will take place.

Registration forms will be sent out this fall to all who have indicated an interest in the Conference. The circular may be viewed on the internet at the following address:

#### http://www.cf.ac.uk/uwcc/chemy/rowlandscc/conf.html

For more information, contact Dr. C.C. Rowlands (Secretary of the Committee of the ESR Group, Royal Society of Chemistry) Dept. of Chemistry, Univ. Wales, Cardiff, P.O. Box 912 Cardiff CF1 3TB, UK; e-mail: saccr@cardiff.ac.uk. More program information can be found in Vol. 8 No. 1.

# FIFTH MEETING of the INTERNATIONAL SOCIETY OF MAGNETIC RESONANCE IN MEDICINE (ISMRM), April 12-18, 1997, Vancouver, British Columbia, Canada.

The 1997 Scientific Meeting of the International Society for Magnetic Resonance in Medicine will combine traditional and new elements of interest to both basic scientists and clinicians to provide a program to appeal to all attendees. Programs will include:

Weekend Educational Programs: Introductory and Advanced MRI: Techniques with Clinical Applications (April 12-13); Progressive Magnetic Resonance Spectroscopy (April 12-13); The Cutting Edge in Spectroscopy (April 13).

**Plenary Lectures:** The plenary lectures will be given on Monday through Friday mornings. Of particular interest is the opening session, which will consist of the Oxford Lecture on the History of MR delivered by Robert Pound. Other plenary lectures will include:

Historical Perspectives of Biomedical NMR: from Basic Physics to Physiology and Diagnosis: Toward Better Understanding of Human Disease (R. Shulman); Celebrating 25 Years of Innovation (W. Edelstein); Clinical MR Imaging: The Ultimate Diagnostic Tool (W. Bradley).

Vascular MR: Vascular Disease—a Surgeon's Perspective (C. Zarins); Methodology of MRA (D. Parker); MRS in Diagnosis (M. Prince).

MR Imaging of Cartilage: Detection of Sports-Related Cartilage Abnormalities (M. Recht); Pitfalls, Pulse Sequences and Quantitative Techniques (C. Peterfy); Cartilage Structure and Pathobiology: Practical Applications (D. Burstein).

Ischemic Heart Disease: MRS for Understanding Ischemic Heart Disease (R. Weiss); The Clinical Role of MRI in Ischemic Heart Disease (A. de Roos); Cardiac MRI Methods—Present and Future (G. Laub).

Funcional MRI: Clinical Impact, Pitfalls and Potential: Neurology: Diagnosis, Prognosis and Rehabilitation (S. Zeki); Psychiatry: A New Patient Population to Image (D. Weinberger); Surgery\Radiotherapy: A Functional Road Map (M. Raichle).

## OXFORD INSTRUMENTS

Supporter of the International EPR Society

#### EPR Cryostats

Cryostats designed specifically for X and Q band EPR experiments

- Helium and nitrogen cooled version available
- Efficient use of cryogen
- Temperature range 1.8 300 K standard (higher temperatures available on request)
- Temperature stability ± 0.1 K

## Teslatron<sup>H</sup>

Compact high homogeneity Teslatron systems for high field EPR and other applications

- Automated magnetic field and temperature control
- Applied fields from 7 to 20 Tesla
- 10 ppm and 1 ppm homogeneities available
- Integration of experiments using National Instruments LabVIEW<sup>®</sup>
- Available in ultra low-loss cryostats for greatest cryogen efficiency
- Choice of room temperature access or integral variable temperature insert

Call us now for copies of our Teslatron<sup>H</sup> and ESR product guides

Oxford Instruments
Scientific Research Division
Research Instruments
130A Baker Avenue
Concord, MA 01742 USA
Tel: 1-508-369-9933

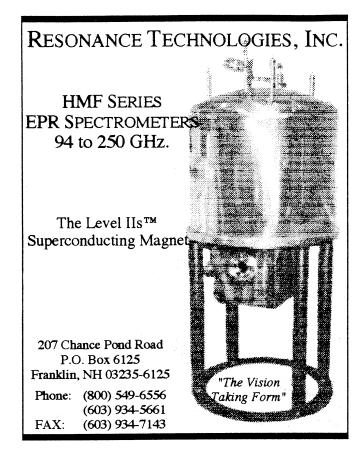
Fax: 1-508-369-6616 E-mail: epr@oxinst.co.uk



Clinical Categorical Courses: Mini-Categorical Courses from April 14-18: Head and Neck Imaging; Diffusion/Perfusion. Clinical Courses: MR Physics and Techniques for Clinicians (April 14-17); The Economics of MRI: A Worldwide Perspective (April 15); Hot Topics for Practicing Radiologists (April 16).

The abstract deadline is November 19, 1996. Abstract forms and other meeting information can be received by contacting ISMRM at info@gateway.ismrm.org.

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA



7th CHIANTI WORKSHOP on MAGNETIC RESONANCE: NUCLEAR and ELECTRON RELAXATION, May 25-31, 1997, San Miniato (Pisa), Italy.

The Chianti Workshops aim to bring together scientists involved in theoretical and experimental aspects of nuclear and electron spin relaxation to study the structure and dynamics of molecules. The Chairpersons are: I. Bertini (Univ. Florence, Conference Chairman) and Z. Luz (Weizmann Inst. Science, Program Chairman). The Organizers are L. Banci (Univ. Florence), E. Gaggelli (Univ. Siena) and C. Forte (C.N.R. Pisa).

For more information, contact one of the following: Z. Luz, Chemical Physics Dept., Weizmann Inst. Science, Rehovot 76100, Israel,  $\blacksquare$ : 972-8-934-2020, FAX: 972-8-934-4123, e-mail:ciluz@wis.weizmann.ac.il; L. Banci, Dept. Chemistry, Univ. Florence, Via G. Capponi 7, 50121 Florence, Italy,  $\blacksquare$ : 39-55-2757550, FAX: 39-55-2757555, E-mail: lucia@risc1.lrm.fi.cnr.it; E. Gaggelli, Dept. Chemistry, Univ. Siena, Pian dei Mantellini 44, 53100 Siena, Italy,  $\blacksquare$ : 39-577-298008, FAX: 39-577-280405, E-mail: gaggelli@unisi.it.

FIFTH INTERNATIONAL WORKSHOP ON ELECTRON MAGNETIC RESONANCE OF DISORDERED SYSTEMS (EMARDIS) and 2nd INTERNATIONAL SEMINAR ON APPLIED EPR, June 8-17, 1997, Sophia, Bulgaria.

Extensive information about these meetings can be found

in the EPR Newsletter (Vol. 7 No. 4).

Further Information. A first circular of both meetings is available. The Organizers request recipients to kindly fill out and return the preliminary registration form included in it 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; **\$\rightarrow\$**: 3592-713-2546 or -3917; telex: 22729 echban, e-mail: NDYEPR@BGEARN.ACAD.BG.

TWENTIETH INTERNATIONAL EPR SYMPOSIUM at the 39th Annual Rocky Mountain Conference, August 3-7, 1997, Denver, CO, USA.

The EPR Symposium will start Sunday evening with an open house at the University of Denver EPR labs, including refreshments provided by Bruker Instruments.

In this Symposium we will emphasize different ways of looking at unpaired electron spins and the complementary information that can be obtained by different techniques. The "normal" CW experiment is most widely used, but it is not necessarily the most powerful way to answer a particular question. There are many other methods including various multiple resonance and time-domain techniques. Since this will be the 20th year for the EPR Symposium we hope to have at least 20 techniques represented.

For further information contact: Prof. Sandra S. Eaton or Prof. Gareth R. Eaton, Dept. of Chemistry and Biochemistry, Univ. of Denver, Denver, CO, 80208-2436, USA. **3**33-871-3102; FAX: 303-871-2254; E-mail: seaton@du.edu.

THIRD EUROPEAN ESR MEETING, August 25-29, 1997, Leipzig, Germany.

The title of this meeting is "Modern Aspects of Structure and Dynamic Investigations of Paramagnetic Systems by EPR". A list of topics for this meeting can be found in the EPR Newsletter, Vol. 7 No. 4.

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; \$\frac{1}{2}\$: 49-341-235-2630; FAX: 49-341-235-2317; E-Mail: beckert@mpgag.uni-leipzig.de.

SECOND INTERNATIONAL CONFERENCE on BIORADICALS and FIFTH INTERNATIONAL WORKSHOP on ESR(EPR) IMAGING AND *IN VIVO* ESR SPECTROSCOPY, October 12-16, 1997, Yamagata, Japan.

The conference will treat all aspects of bioradicals, with special attention to ESR spectroscopy. The following subjects comprise the main scientific scope:

- A. Bioscience of reactive oxygen species including Chemistry, biochemistry and pathophysiology of bioradicals; Redox regulation and signal transduction; Antioxidants and food science
- B. Biological applications of ESR spectroscopy, e.g., ESR imaging; *In vivo* applications of ESR;

Publication of the International EPR(ESR) Society

Biological applications of ESR methodologies

C. Other topics to be determined

To receive a circular, contact Dr. Hiroaki Ohya-Nishiguchi, Institute for Life Support Technology, Yamagata Technopolis Foundation, 2-2-1 Matsuie, Yamagata 990, Japan; **\$\sigma\$**: 81-236-47-3134; FAX: 81-236-47-3149; E-mail: ohya@ymgt-techno.or.jp.

FIFTH INTERNATIONAL CONFERENCE ON SPIN CHEMISTRY, October 26-31, 1997, Jerusalem, Israel.

An official circular will be available shortly. For more information please contact Haim Levanon, Dept. Physical Chemistry, The Hebrew University, Jerusalem, 91904 ISRAEL. **2**: 972-2-658-5544; FAX: 972-2-618-033; e-mail: levanon@vms.huji.ac.il.

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

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

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

For further information on the XVIIIth ICMRBS, please contact Prof. M. Kainosho, Dept. Chemistry, Tokyo Metropolitan Univ. (TMU), Hachioji, Tokyo, Japan; \$\frac{1}{2}\$: 81-426-77-2544; FAX: 81-426-77-2525; e-mail: kainosho@raphael.chem.metro-u.ac.jp.

## FROM EPR CENTERS

EPR Center for the Study of Viable Biological Systems at Dartmouth Medical School, Hanover, NH USA

As we were going to press, we learned that this center is established starting September 30, 1996, with initial funding for five years. This is now the fourth EPR Center funded by the National Center for Research Resources, NIH. The new Center, with Hal Swartz as director and Ted Walczak as Co-Director, will continue their work in the development and application of EPR techniques for studies in functional biological systems, especially in vivo EPR spectroscopy. This independent EPR Center is a direct descendent of the Illinois EPR Research Center at the University of Illinois and a longer term descendent of the National Biomedical ESR Center at Milwaukee. The contact numbers and addresses, etc. are listed in the Newsletter masthead (page 23), along with those of the other NIH-supported EPR Centers.

Establishment of this center opens several potential positions, which are immediately available; see "Positions Available" below. We wish this new center every success!

# POSITIONS AVAILABLE & WANTED

## **POSITIONS AVAILABLE**

Research Associates/Post-doctoral Positions at the EPR Center for the Study of Viable Biological Systems. The EPR laboratory at Dartmouth has several immediately available openings for research and development in the EPR Center and/or in the program project for the development and application of oxygen-sensitive paramagnetic materials. The opportunities/needs range from instrumental development of low frequency EPR spectroscopy to biological applications in animals to studies in isolated cell systems. There are specific needs for individuals with strong backgrounds in engineering/instrument development and for an individual with excellent skills in cell culture. The initial appointments will be made for 1 year with the possibility of extensions up to 5 years or longer. Candidates should submit a complete CV including a description of prior experience and areas of research interests, and should arrange for 3 letters of reference to be sent directly to Prof. Hal Swartz, Dartmouth Medical School, 7785 Remsen, Hanover, NH, 03755 USA; e-mail: harold.swartz@dartmouth.edu; FAX: 1-603-650-1130.

Research Assistant in Electron Paramagnetic Resonance. The Department of Chemical Engineering at the National University of Singapore invites applications for a research assistant position. The successful candidate will be involved in a research program of investigating electron transport through liquid membranes with redox active properties. Fluent English and knowledge of EPR is a plus. Preference will be given to a candidate holding a Ph.D. (or equivalent) in physical chemistry/biochemistry or related fields, although persons with M.S. degree are also welcome to apply. Initial appointment will be made for a half or one year with a potential renewal. Level of compensation will be in accordance with qualification of the candidate. Candidates should submit a curriculum vita and arrange for three letters of reference to be send to: Dr. Nikolai Kocherginsky, Department of Chemical Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore, 119260. (65)7715083, FAX (65) 7791936 E-mail: Chenk@leonis.nus.sg.

Visiting Woman Professor. We can offer a temporary visiting professorship for a woman scientist with a background in EPR. The position is for 12 months. Costs, up to 0.85 MSEK or \$125,000 will be covered by a grant from the Swedish National Science Research Council. The grant can be used for salary and travel. At present the research is focused on structural and dynamical

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

investigations of radical ions, in matrices and on surfaces, of the structure of paramagnetic species in Cu-exchanged zeolites, and structural and dynamic studies of protein folding using spin labels. In addition some single studies of radiation damage are performed as well as studies of EPR dosimetry. The research can be in any of these or other fields proposed by the candidate, subject to limitations set by available equipment. We have at present a CW Bruker 200 EPR and ENDOR spectrometer and will have a Bruker 380 pulsed EPR and ENDOR spectrometer installed at the end of 1996. Please contact Anders Lund for further information: Dept. Physics and Measurement Technology, Linkoping Univ., S-581 83 Linkoping, Sweden; ph: 46-13-282665; FAX: 46-13-132285; e-mail: ald@ifm.liu.se; World Wide Web: http://www.ifm.liu.se/Chemphys.

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 negotiable starting date. 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.

#### **POSITIONS WANTED**

EPR spectroscopist seeks academic or industrial position. Physical chemist, now postdoctoral fellow in Chemistry Dept., Univ. Houston. Education: 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 Dept., Univ. Of Houston, Houston, TX 77204-5641, USA; **2**: 1-713-743-3251; FAX: 1-713-743-2709; e-mail: wasowicz@jetson.uh.edu or wasowicz@orange.ichtj.waw.pl.

## **EOUIPMENT & SUPPLIES** *EXCHANGE*

#### FOR SALE: 100KC SPECTROMETER

Will sell at best offer: 100KC spectrometer manufactured by Alpha Scientific Laboratories, ALX-10X band (V-58C Varian Reflex Klystron). The magnet has 12" diameter poles and weighs 6,000 lbs. (turntable mounted). The unit is complete except for the EPR cavity, and a set of schematic diagrams is included. Please contact John Ledlie, CompuWorks, Columbia, SC 29201, USA; 2: 1-803-799-2762; FAX: 1-803-799-1524; e-mail: ledlies@scsn.net

#### 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; knight lon/furman@furman.edu.

#### **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 dipas@jeol.com.

#### OFFERED: HELP IN THE DESIGN AND CONSTRUCTION OF EPR ELECTRONICS

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 KHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a conversion kit to convert Varian field control units to voltage-controlled scan operation. A 6 digit 1 ppm frequency counter is available in X-, C-, S- or L-band or Megahertz versions. Complete microwave/RF bridges from 150 MHz to L-, S-, or C-band are available from designs previously built and tested at the University of Denver. Contact: Richard W. Quine, **\(\mathbb{\pi}: 1-303-871-2419\)** or e-mail: rquine@du.edu.

#### FOR SALE: VARIAN SYSTEM

Resonance Instruments presently has available:

- 1) a E110 Q-band Bridge with cavity
- 2) replacement Klystrons for Varian EPR Bridges (at reduced prices)
- 3) Model V4533 VARIAN EPR TE011 mode, rotating cylindrical cavity
- 4) VARIAN general purpose cavity E2315) VARIAN V4500-41A low/high power microwave bridge with new klystron—excellent condition

Publication of the International EPR(ESR) Society

6) X-band DEWAR probe outfitted with a tuner and with stainless steel waveguide

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

#### **AVAILABLE: TWO IBM9000 COMPUTERS**

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

FAX: (510) 642-2069; E-mail: weber@garnet.berkeley.edu; www: http://www.mse.berkeley.edu/faculty/weber/weber.html

#### WANTED: USED X-BAND MICROWAVE BRIDGE

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

## **ANNOUNCEMENTS**

#### MAILING LISTS FOR SCIENTIFIC MEETINGS

If you are planning a scientific conference, you may contact an officer of the IES or the IERC (address at left) to obtain a list of the 1,400+ Society members for use in issuing invitations. If you would like mailing labels, Martha Moore, who provides secretarial support for the Society, can do this at cost -- approximately \$50.00 per 1,000 (includes cost of labels, postage and, if you wish, a disk copy of the list in ASCII format). Labels for the entire database (over 3,800 members and non-members) would cost about \$200.00.

#### MEMBERSHIP INFORMATION AVAILABLE ON THE WEB

This year, a list of all members whom the IES records show as having paid dues in 1994, 1995, and/or 1996 was put 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 update the list monthly; please allow time for recent payments to be placed on the list. 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 dues payment form is on this web site along with methods to pay dues, depending on where in the world you are located.

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

#### ABOUT THIS PUBLICATION

- This publication is the official newsletter of the International EPR(ESR) Society. It is supported by the Society, by corporate and other donors, and by the Biomedical Technology program of the Division of Research Resources in the U. S. National Institutes of Health through the Illinois EPR Research Center at Urbana.
- •Editor: R. Linn-Belford
- •Assistant Editor, Becky Gallivan
- Typography: Martha Moore.
- The EPR Newsletter is produced with the cooperation of these 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.

**2**: 414-456-4008. FAX: 414-266-8515.

E-Mail address: cfelix@post.its.mcw.edu

WWW: http://www.biophysics.mcw.edu/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 address: peisach@aecom.yu.edu

WWW: http://spin.aecom.yu.edu

## EPR Center for the Study of Viable Biological Systems,

Prof. Hal Swartz, Director

Prof. Ted Walczak, Associate Director

Dartmouth Medical School, Dept. of Radiology 7785 Remsen, Hanover, New Hampshire 03755-3863, USA.

**☎**: 603-650-1784. FAX: 603-650-1130.

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

Illinois EPR Research Center (IERC),

Prof. R. Linn Belford, Director; Prof. Robert B. Clarkson, CoDirector; Prof. Peter G. Debrunner, Assoc. Director, Prof. Mark J. Nilges, Asst. Director, Prof. Alex I. Smirnov, Laboratory Manager; Ms. Becky Gallivan, Asst. to the Directors; Ms. Martha Moore, Secretary.

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

#: 217-244-1186. FAX: 217-333-8868.

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

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

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

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

Volume 8, Number 3

Page 1

Fall/Winter, 1996

## 1996 IES Silver Medals—

At the 1996 International EPR Symposium, July 21-25 in Denver, Dr. Ronald Mason was presented with a certificate to acknowledge his outstanding work which led to his selection as the 1996 Silver Medal Awardee in biology and medicine. Prof. Klaus Möbius was presented with a certificate acknowledging his stellar contributions in EPR applied to chemistry. President of the Society, Keith McLauchlan, Dean of Chemistry, Oxford, UK personally presented the certificates and also presided as host at a special awards banquet to honor all 1996 IES awardees.

### Dr. Ronald Mason: Biology & Medicine

It gives me great pleasure and satisfaction to write this



piece on behalf of Dr. Ronald Mason, the recipient of the 1996 IES Silver Medal Award for Biology and Medicine. After receiving mу Ph.D., under the direction of Prof. Lowell Kispert at the University of Alabama, I joined Ron Mason at NIEHS in 1978 as his first postdoctoral

Mason at IES Award Symposium

visiting fellow. Even after all these years, we still collaborate and write papers together.

Ron did his Ph.D. work with Prof. Harriman of the University of Wisconsin, Madison. He received postdoctoral training in Prof. Freed's laboratory, where he learned very sophisticated and useful aspects of advanced ESR spectroscopy. He then spent five years as a Research

(Ron Mason ... continued on page 2)

- Editor: R. Linn Belford, Urbana, IL
- Assistant Editor, Becky Gallivan, Urbana, IL.
- Typography: Martha Moore, Urbana, IL.
- This, the official newsletter of the International EPR(ESR) Society, is supported by the Society, by corporate and other donors, and by the Division of Research Resources in the U.S. National Institutes of Health. For additional information including how to contact the editor, see the box "About This Publication" on p. 26.

#### FELLOWS OF THE INTERNATIONAL EPR(ESR) SOCIETY

- ANATOLE ABRAGAM
- GEORGE FEHER
- BREBIS BLEANEY
- CLYDE HUTCHISON, JR.
- RALPH HAHN
- . J. H. VAN DER WAALS ALEKSANDR PROKHOROV • SAMUEL WEISSMAN

### Professor Klaus Möbius: Chemistry

The contributions of 1996 Silver Medalist Klaus Möbius

to the field of EPR a n d ENDOR spectroscopy physics, chemistry, and biology have been internationally recognized and most highly esteemed over the last 25 years. Some outstanding examples of his highly original work are:

The extension of ENDOR-in-solution high-power electron-nuclear-nuclear triple resonance in the two versions, Special TRIPLE and General TRIPLE, to hyperfine couplings



measure and assign Möbius at IES Awards Banquet

of complex bioorganic molecules. These very powerful (Klaus Möbius ... continued on page 2)

IN THIS ISSUE	
IES Silver Medals, 1996 (Ron Mason; Klaus Möbius)	1-2
International EPR(ESR) Society Affairs	2-9
From the Editor (R. L. Belford), From the President (J.Norris),	- 74
Fellows (Abragam, van der Waals, Bleaney, Hahn), Langmuir	
Award (Freed), IES Officers, Zavoisky Award (Feher)	
The Computer Corner (K. Madden)	9-11
	1-15
High-field EPR (T. Prisner)	
- 이유성하다 F '유럽 전통 이유 : (1. 2. 1. 1. 2. 1. 1. 1. 2. 1. 2. 1. 2. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.	5-16
	6-18
	8-19
Company Profiles 1	9-21
Notices of Meetings	21-23
Positions Available & Wanted	23-25
Equipment & Supplies Exchange	
Announcements (Mailing lists; Info. on WWW; E-mail updates)	. 26
About this Newsletter (The Masthead)	26
IES Corporate Sponsors	27
Appendices: IES Information and Registration Forms	
BALLOT FOR COUNCIL MEMBERS—Please mark and return!	

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

(Ron Mason—continued from page 1) ····

Chemist in Jordan Holtzman's laboratory in Veteran's Administration Minneapolis, where he became thoroughly exposed to the possibilities of applying sophisticated ESR techniques to biological problems in pharmacology and metabolism. In 1978 Ron joined the National Institute of Environmental Health Sciences, Research Triangle Park, where he is now group leader of the Free Radical Metabolite Program.

Ron Mason was primarily responsible for rekindling the interests of Pharmacologists and Toxicologists in Free Radicals in Biology. Early on, Ron wrote several superb Reviews on "The detection of free radical metabolites from drugs and xenobiotics" which linked several interdisciplinary areas and opened new opportunities for ESR in biological systems, both *in vitro* and *in vivo*. Free Radical Symposiums became part of the FASEB and SOT annual mettings. The ESR techinique gained more recognition among free radical biologists. Ron's relentless pursuit to increase the awareness of free radical researchers in ESR is clearly paying off. For example, in the Oxygen 96 meeting to be held in Miami, there will be an ESR workshop organized by Ron that is to run the whole day prior to the regular meeting.

From a scientific point of view, Ron is probably the only famous ESR person, to my knowledge, with thorough expertise in both spin labeling and spin trapping techniques. His contributions on nitroanion radicals and their futile aerobic metabolism are clearly text book materials. Another highlight of Ron's research activities is the *in vivo* detection of spin adducts from a variety of toxic inorganic and organic chemicals, including many metals and drugs. His recent publications on site-directed spin trapping in heme-proteins should open new avenues for biological spin trapping. Over the years, Ron has been exceptionally productive. His *curriculum vitae* includes more than 200 peer-reviewed papers and 75 reviews. Even by Freed's calculation this is not a small number!

In conclusion, I am honored to write this piece on Ron - The Renaissance Man of Free Radicals in Biology.

B. Kalyanaraman, Medical College of Wisconsin, USA

(Klaus Möbius—continued from page 1) ....

spectroscopic methods for complex systems are now commonly applied, even by using commercial instrumentation;

- ENDOR in liquid crystals to measure tensorial hyperfine and quadrupolar interactions in radical solutions;
- CIDEP-enhanced ENDOR to measure, by time-resolved methods, hyperfine interactions in transient photoproducts;
- High-field/high-frequency EPR and ENDOR at microwave frequencies as high as 95 GHz (W-band) to resolve small g-factor anisotropies and hyperfine tensor components in large biomolecules involved in primary photosynthesis.

Over the last decade, his research has been focused on X-band ENDOR/TRIPLE resonance and W-band EPR/ENDOR spectroscopy of the primary donor and acceptor ion radicals and triplet states of various bacterial photosynthetic reaction centres in fluid and frozen solution as well as in single crystals.

More recently, by applying cw and time-resolved EPR spectroscopy at X- and W-bands, Klaus Möbius and his collaborators obtained detailed structural and dynamic information about the co-factors involved in native photosynthetic and biomimetic electron transfer reactions, for instance; about the primary donor cation, the primary acceptor anion, and the spin-correlated coupled ion radical pairs. These experiments provided details of the spatial and electronic structure of complex molecules and their interactions with their environment. They will certainly contribute to a better understanding of the structure-function relationship in vectorial photosynthetic electron transfer. In a more general statement it must be emphasized that the work of Klaus Möbius has to be considered as excellent by all standards and that it is internationally highly recognized by the magnetic resonance community. This is illustrated by impressive academic awards and honors he has received since 1966 (e.g. Karl-Scheel Award of the Physikalische Gesellschaft zu Berlin, Bruker Lecturer Award of the Royal Society of Chemistry, Max-Planck-Research Award, International Zavoisky Award, Philip-MorrisForschungspreis 1996).

The scientific work of Klaus Möbius over the years is characterized by his openness for interdisciplinary teamwork, e.g. with groups from chemistry, with students and postdocs and for cooperation between scientists from all over the world to the benefit of human relations.

Personally, the author of this laudatio wants to thank Klaus Möbius for a longstanding friendship and for enthusiastic involvement in our joint research projects lasting for more than two decades.

Harry Kurreck, Freie Universität Berlin, Germany

## **♦ IES AFFAIRS ♦**

ANNOUNCEMENTS AND
REPORTS FROM THE INTERNATIONAL
EPR SOCIETY

#### From the Editor—

It is time again to remind our readers that the Society and the Newsletter could not continue without the support of all of our corporate members. We should appreciate their support, and the most telling expresssion of our appreciation would be to do some business with them whenever possible. I extend a hearty welcome to two new corporate supporters of the International EPR (ESR) Society — Oxis International and Resonance Instruments! Clarence Arnow, the President of Resonance Instruments, has a long record of support for

Publication of the International EPR(ESR) Society

our activities through his fomer company, Micro-Now, and is well known to many of us in the EPR community. We wish him well in his new venture.

I am also happy that in this issue we are able to provide short essays about several distinguished IES Award winners - Silver Medalists and Society Fellows. As well as being fine scientists, they are all interesting human beings, and I think we all enjoy learning a bit more about them.

R. Linn Belford, Editor

## From the President—

One of my first duties as President of the IES is to thank my predecessors on behalf of the International EPR Society (IES). Although I am amazed at the quick prosperity of the IES, the success is clearly the result of the work and skills of the first two Presidents of the Society and their fellow officers. The founding President Hal Swartz got us off to a great start. Then Keith McLauchlan built the Society up to its present membership. In a span of eight years the Society has grown from ground zero to almost 1500 members, really an astonishing feat. Under the leadership of these two people the Society currently presents awards for outstanding performance and service in EPR, maintains a very useful membership directory and publishes this newsletter (thanks to the Illinois EPR Research Center and its staff).

As President of the IES I would like to encourage all members to participate in the Society's award processes. Please note that the procedures for nominating candidates for awards and honors are described routinely in these newsletters, and in particular, in this newsletter.

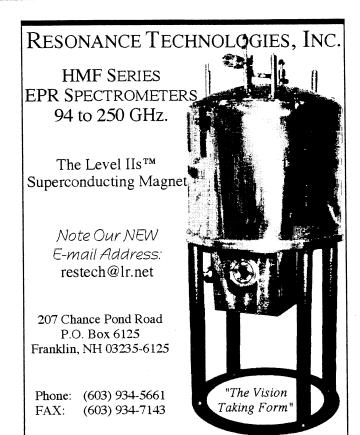
It is my hope that the Society will continue to grow and contribute more and more to the cause of EPR and science worldwide. I am truly fortunate in having an outstanding group of fellow officers to guide us into the future. To remain really successful, the membership must participate. I therefore encourage each of you to express any new ideas or comments to one of the officers or to me. For example, if there are services or functions that the Society should consider or modify, please let one or more of us know. Finally, I wish everyone and the Society a most successful new year for 1997.

Jim Norris

## Professor Anatole Abragam: IES Fellow, 1995

Anatole Abragam was born on 28 December 1914 in Moscow, where his mother, one of the first women to qualify as a medical doctor, practised both before and after the first world war. With Anatole and his older sister, she moved to Paris in 1925, followed by her husband in 1936. Anatole arrived without a word of French, so that "he spoke it straightaway without any foreign accent".

After attending the University of Paris and the École Supérieure d'Electricité, Anatole came to Oxford in 1948, where I met him because Maurice Pryce, the Wykeham



Professor of Theoretical Physics, assigned him the theory of electron paramagnetic resonance as the topic for his doctorate of philosophy, gained in 1950.

Returning to France, employed by the Commissariat à l'Énergie Atomique, he became head of the Magnetic Resonance Laboratory (1955), of Nuclear and Solid State Physics (1959), and Director of Research (1971-80). He was Professor of Nuclear Magnetism at the Collège de France (1960-1985), and President of the French Physical Society in 1967.

His spectacular achievements include the invention of the "solid effect", and the development of highly polarized nuclear targets; application of the technique of "adiabatic demagnetisation in the rotating frame" to produce ordered assemblies of nuclear spins at both positive and negative temperatures. After developing the concept of "pseudomagnetic moments" of nuclei, he measured these moments by scattering polarized neutron beams from highly polarized nuclear targets.

Amongst his numerous honours, he is a Foreign Member of the Royal Society of London, and an Honorary Fellow of Merton and Jesus Colleges (Oxford). This year he received the Lomonosov Gold Medal, the highest award of the Russian Academy of Sciences.

His hobbies are music, walking in the countryside, listening to tapes of Shakespeare's plays.

Brebis Bleaney University of Oxford



## **Professional Societies & Publications**

500 Sunnyside Boulevard Woodbury, NY 11797-2999 USA Phone: 1-516-576-2411 Fax: 1-516-576-2481

#### Prof. Joan H. van der Waals: IES Fellow 1996

Joan van der Waals is one of the pioneers of ESR spectroscopy on photo-excited triplet-state molecules. In 1958 he was the first to discover the " $\Delta m$ =2" transitions and demonstrated that these transitions hardly show any anisotropy. Hence they can be observed in a rigid solution of randomly oriented molecules in a glassy matrix. This solved the problem of finding suitable host materials for the molecules to be studied and this discovery paved the way for a whole field of research on triplet state molecules.

A very important contribution made by van der Waals was the observation and explanation of the selection rules for the population and depopulation of the sublevels of the triplet state of aromatic molecules. This opened the possibility for Optical Detection of Magnetic Resonance (ODMR) spectroscopy in the presence as well as in the absence of a magnetic field. This technique has been developed by him and his collaborators into a means for determining the kinetic properties of the individual spin levels of the triplet state. As a culmination of this work, he and his group carried out an experiment in which the coherence between the two sublevels of the triplet state could be observed as a quantum beat in the phosphorescence emission.

Around 1971 van der Waals realized that his research group was in a favourable position to study the electronic structure of porphyrins. Well-known examples of porphyrin derivates are chlorophyll and bacteriochlorophyll in photosynthesis and haemoglobine in the respiration chain. By dissolving porphyrins in single crystals of n-alkanes and applying the newly developed ODIVIR technique, highresolution laser spectroscopy and ESR he was able to solve many of the fundamental problems related to the electronic structure of porphyrins. Several ODIVIR and ESR experiments on photosynthetic bacterial reaction centres were carried out in his laboratory and were largely inspired by his interest and imagination. In the last years of his professional career his attention turned to the tetroxo anions of the do transition metals. He and his students identified the lowest triplet states of a number of these ions like Cr<sub>2</sub>O<sub>7</sub><sup>2</sup>, VO<sub>4</sub><sup>3</sup>, Mo0<sub>4</sub><sup>2</sup>, employing ESR and ODIVIR techniques at frequencies up to 75 GHz.

Joan van der Waals retired in 1989 but is still very active as a member or chairman of advisory committees serving the scientific community in the Netherlands. Sailing is still his great hobby. Sometimes this leads to the curious situation that he is late for a meeting because of lack of wind. This however never had a negative influence on the quality of his reports to these committees!

Jan Schmidt Leiden University

### Professor Brebis Bleaney: IES Fellow 1995

Although Brebis Bleaney is best known for his pioneering work on electron paramagnetic resonance (EPR), he has made several distinct contributions to physics in his long, active career: he is now still publishing frequently at age 81. He has also worked, in chronological order, on: the thermodynamic temperature scale in the liquid helium region, sources and applications of microwaves (in World War 11), microwave spectroscopy of gaseous ammonia, nuclear alignment, atomic beam spectroscopy, enhanced nuclear magnetism and enhanced nuclear magnetic resonance. However, his greatest innovation was EPR performed at microwave frequencies, independently of the simultaneous lower frequency work of Zavoisky. By working at temperatures down to the liquid helium range he was able to examine EPR of 3d and 4f ions with too rapid spin-lattice relaxation for observation at room temperature; and by working in mixed crystals of isomorphous paramagnetic and diamagnetic salts, he was able to obtain narrow lines and measure fine and hyperfine structures to great precision. This work led to a detailed understanding of the paramagnetism, crystal fields and spin-lattice relaxation of 3d and 4f ions in crystals. Bleaney's interest in hyperfine structure led him independently to the idea of ENDOR.

In addition to being a fine experimentalist, Bleaney had a great appreciation of theory, and he has been able to bridge the gap between professional theorists and experimentalists. His close collaboration with Pryce and Abragam led to the concept of the spin hamiltonian; and he was instrumental in launching the theoretical careers of Ken Stevens, Roger Elliott, Mary O'Brien and Brian Judd.

Bleaney was not only an inspired researcher, he was also an inspiring tutor of physics at St John's College in Oxford. He has a wide appreciation of physics which enabled him to be a frequent and constructive maker of comments at conferences and colloquia. He has written two important text books on "Electricity and Magnetism" with his wife Betty, and "Electron Paramagnetic Resonance of Transition Ions" with Anatole Abragam.

Bleaney is a devoted family man. He married Betty Plumpton, one of his earliest research students. Playing with son and daughter was for many years listed as one of his hobbies in "Who's Who". He has always treated his graduate students as part of his extended family. When he was Dr Lees' Professor at the Clarendon, his friendly influence was spread more widely over a range of colleagues, graduate students and postdocs in physics. He has always enjoyed tennis, and still at 81 is capable of sustaining a long set, and beating many of his younger colleagues.

Publication of the International EPR(ESR) Society

Bleaney is appreciated in Oxford for his wide humanity and warm friendliness, as well as for his brilliant science which helped to put the Clarendon Laboratory on the map. In its heyday, the Clarendon was the major centre of electron magnetic resonance in the West, and the young people who were Bleaney's satellites have moved off to make important contributions in their own orbits, having learned from a stimulating teacher, a tolerant and encouraging supervisor and a warm and supportive colleague.

Michael Baker University of Oxford

## Professor Erwin L. Hahn: IES Fellow 1996

On the occasion of his election as a Fellow of the Society, it is indeed a great privilege and pleasure for me to write some words about my mentor, colleague and dear friend, Erwin L. Hahn, one of the giants of modern physics.

A brief history—Hahn was born in Sharon, Pennsylvania in 1921. He had several possibilities for a career, among them the Navy, movie star, and musician (many of us are aware that Hahn is an enthusiastic and gifted violinist). Well, we can be thankful that he turned toward science, in particular that he chose magnetic resonance and optics. He received his Ph.D. in Physics from the University of Illinois. He was a Research Associate at the University of Illinois, a National Research Council Fellow at Stanford University where he worked with Felix Bloch, and a Research Physicist at IBM Watson Scientific Computing Laboratory before he came to Berkeley, where he has been on the faculty since 1955. In addition to his famous published works, Hahn has always been a brilliant, provocative and entertaining lecturer.

Hahn is the discoverer of the spin echo, a phenomenon of monumental significance in many areas of science. The occurrence of such time-reversal phenomena has important implications in the statistical physics of processes which appear to approach equilibrium, and echoes were the first manifestation of the infamous "Loschmidt-Boltzmann Paradox." Using spin echoes, Hahn discovered the indirect or scalar coupling of nuclear spins via hyperfine interactions. The use of spin echoes has also featured prominently in magnetic resonance imaging, one of the most important developments in medical diagnostics in recent decades.

It was Hahn who also obtained the first nuclear quadrupole resonance echoes in solids and he is co-author of

a definitive and widely quoted text on nuclear quadrupole resonance spectroscopy. With his students, he introduced the idea of double resonance in the rotating frame, a technique that allowed for the first time the detection of NMR for rare nuclear spins, and is widely used today by solid-state physicists and chemists.

In the area of coherent laser physics, Hahn and coworkers predicted and demonstrated "Self-Induced Transparency," in which coherent optical pulses of particular shapes and areas propagate unattenuated through an otherwise resonantly absorbing medium. He provided a full theory using coupled Maxwell and Bloch equations for the phenomenon, together with experimental examples. This effect, a clear-cut manifestation of a many-particle vortex interaction, is known as a soliton. Its existence in other cooperative and statistical phenomena is the subject of much current research.

My own first indirect association with Hahn involved an experiment that Won-Kyu Rhim and I did with John S. Waugh at MIT concerning the free-induction decay of coupled spins in a crystal. The question then was whether the decay of magnetization under this complex Hamiltonian was really irreversible. It turned out that you could, by applying an extended sequence of pulses *after* the total decay of order, bring back the magnetization. About that time, Waugh was going out to California and he planned to drop in on the Father of the Spin Echo and tell him about our work. When he came back from the trip and I asked him what Hahn had to say, he replied that Hahn had remarked "With that many pulses I could bring back the Messiah."

My official acquaintance with Hahn began about twenty-five years ago when I was awarded a Miller Fellowship in physics to work with him at Berkeley, a relationship that ended prematurely when I accepted a faculty position in chemistry. Since that time, one of the marvels of being at Berkeley has been the privilege of having Hahn as a colleague, scientific collaborator, and partner in humor.

Some years ago there took place a symposium at Berkeley in honor of Hahn's seventieth birthday. Listening to the speakers, among them numerous colleagues and former students of Hahn, one could not help but be astounded by the breadth and depth of his impact as reflected in the generations of scientists whom he has educated and influenced. Telegrams from intimates were read aloud—my favorite one said "Dear Erwin, congratulations. I haven't

## **CPI Sets the Standard for EPR Klystrons**

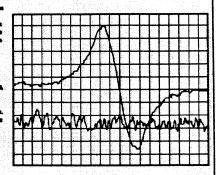
CPI Replacement Klystrons deliver:

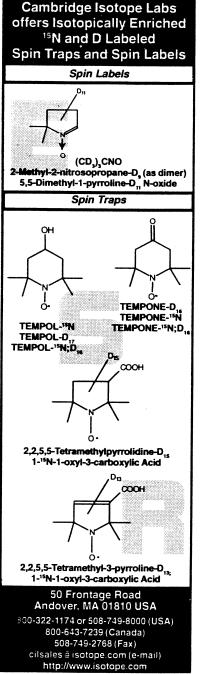
- Optimum application flexibility Long Life
- Reliable performance, low noise New warranty
- X band for Century Series, E lines, plus Q band Now available directly from CPI. For more information call CPI at 1-800-843-8780 or 415-846-3188 from outside the U.S.



formerly a division of Varian@

The plot Blustrained we taken with a Varien west pitch assupte in a TE102 coulty under the conditions specified in the Varien E Line Berice unconflied (E102/E100 bridge) instruction menor in Signal to noise ratio represented in 345-t. J. 2.5 conversion factor was used to convert rum noise to P-P noise The west pitch samply had a .053 meltiplication factor, Without the multiplication factor, the signal to noise would be 300-t.





seen you for many, many years, but you don't look seventy." On that occasion, the Chancellor of the University of California awarded Hahn highest honor. the "Berkeley Citation."

In conclusion, let me that Hahn's contributions to science are phenomenal. He has done so many beautiful things, a fraction of any one of which could serve each of us for a lifetime. To remind us all, and to set things in perspective, just four of his papers involve: Free Precession. Spin Echoes, Double Resonance, and Self-Induced Transparency.

Hahn has been an inspiration for generations of scientists and we owe him a debt beyond words. For me, becoming acquainted with spin echoes and time reversal, and becoming afflicted with the Hartmann-Hahn condition (from which I suffer to this very day) have been an unforgettable part of my scientific education and experience for which I am forever grateful. Certainly, Hahn is a genius, one of the greatest physicists of the

century and, moreover, he is a man of enormous integrity in his scientific and personal life. He has been, and he remains, a shining light for all of us to follow.

Erwin, on behalf of us all in magnetic resonance, I'd like to say thank you, God bless you, and may you have many more happy years of science, music and humor.

> Alexander Pines University of California, Berkeley

## Freed Wins Langmuir Prize

Congratulations to Prof. Jack Freed (Cornell) on winning the 1997 Irving Langmuir Prize in Chemical Physics. The Executive Council of The American Physical Society will present the prize at a banquet on April 20, 1997. The prize was established to recognize and encourage outstanding inter-disciplinary research in chemistry and physics, in the spirit of Irving Langmuir. Prof. Freed is being honored for his development of new magnetic resonance methods and theory, including computational algorithms for the stochastic Liouville equation, time-domain ESR methods for the study of molecular dynamics in liquids, applications of ESR to surface science, and the discovery of nuclear spin-waves in spin-polarized H atoms.

### OFFICERS OF THE INTERNATIONAL EPR(ESR) SOCIETY

Ballots received for the election of officers of the IES have been counted and the persons recommended by the nominating committee have been approved. (There were three write-in names.) We congratulate the new officers and look forward to working with them for the continued growth of the Society. Following please find the list of the elected officers, their addresses, e-mails, etc. should you wish to contact them regarding Society business or just to extend your congratulations. By the rules of the IES Constitution, Past President Keith McLauchlan will now become Chair of the Nominating Committee. Our thanks to Prof. Harold Swartz, Founder-President, who has carried out these duties until now.

Becky Gallivan, Assistant Editor

PRESIDENT: Prof. James R. Norris, Jr., Univ. Chicago, Dept. Chemistry - Searle 133, 5735 S. Ellis Avenue, Chicago, IL 60637-1403 USA; ☎: 1-773-702-7864; FAX: 1-773-702-0805; E-mail: j-norris@uchicago.edu.

VICE PRESIDENT: Prof. Klaus Möbius, Free Univ. Berlin, Dept. Physics, Arnimallee 14, Berlin, D-14195 Germany; **3**: 49-30-8382770; FAX: 49-30-8386046; E-mail: plato@platon.physik.fu-berlin.de.

SECRETARY: Prof. Arthur Schweiger, ETH-Zentrum, Physical Chemistry Laboratory, CH 8092 Zürich, Switzerland; ☎: 41-1-632-4362; FAX: 41-1-632-1021; E-mail: turi@nmr.phys.chem.ethz.ch.

TREASURER: Dr. Balaraman Kalyanaraman, Medical College of Wisconsin, National Biomedical ESR Center, 8701 Watertown Plank Road, Milwaukee, WI 53226 USA; ☎: 1-414-456-4035; FAX: 1-414-266-8515; E-mail: balarama@post.its.mcw.edu.

FOUNDER PRESIDENT: Prof. Harold M. Swartz, Dartmouth Medical School, Department of Radiology, 7785 Remsen Bldg. #600D, Hanover, NH 03755-3863 USA; **2**: 1-603-650-1955; FAX: 1-603-650-1130; E-mail: harold.swartz@dartmouth.edu.

Publication of the International EPR(ESR) Society

## Feher Wins 1996 Zavoisky Award

Following the extensive nominations from the International Community of EPR scientists the International Zavoisky Award Committee is delighted to announce that the 1996 Zavoisky Awardee is Professor Dr. George Feher (La Jolla). He was awarded the Prize at the annual Development of Workshop "Modern Paramagnetic Resonance" held in Kazan, 18-22 September 1996. Prof. Feher, a Gold Medalist of the IES, is distinguished for his work in electron paramagnetic resonance and, in particular, his contribution to the development of magnetic resonance in solid-state physics and photosynthesis research. For more information, please refer to a further citation of his work which will appear in a forthcoming issue of "Applied Magnetic Resonance".

Professor Kev M. Salikhov Chairman of the Zavoisky Award Committee

# Laudatio for Professor Dr. George Feher on the Occasion of His Receiving the Zavoisky Award

The Zavoisky Award is presented to Professor Feher in recognition of his outstanding contributions to knowledge in physical and biological sciences, in paricular to the field of magnetic resonance in solid-state physics and photosynthesis research. The originality of his work has been apparent over the last 35 years and clearly puts him into the frontier line of research in physics, biophysics and biology. Outstanding examples of this highly esteemed work are the development of the Electron Nuclear Double Resonance (ENDOR) technique in 1956, a technique most successfully applied now in solid-state physics, molecular physics, chemistry and biology, and his contributions to the understanding of fundamental processes in bacterial photosynthesis on the molecular level.

His name is related to several milestone achievements in photosynthesis research, for instance:

- the first isolation and characterization of bacterial reaction centers in 1970/71;
- the identification of the primary donor as a dimer of bacteriochlorophylls by EPR and ENDOR in the early 70's (independent from the parallel discovery by J.R. Norris, Argonne);
- the crystallization and subsequent X-ray structure determination at atomic resolution of the reaction center of the purple bacterium Rb. sphaeroides (shortly after this had been achieved for Rps. viridis by H. Michel, J. Deisenhofer, R. Huber (Nobel prize 1988 for chemistry)) and, more recently;
- the improvements in understanding the structure-function relationship in vectorial electron transfer in photosynthesis by combining site-directed mutagenesis, X-ray crystallography and ENDOR techniques.

It is this continuous high-calibre scientific productivity of Dr. Feher over the last 35 years that is most convincing, with highlights in EPR/ENDOR on donors and acceptors in bacterial reaction centers, X-ray crystallography, electron

## OXFORD INSTRUMENTS

Supporter of the International EPR Society

### **EPR** Cryostats

Cryostats designed specifically for X and  $\Omega$  band EPR experiments

- Helium and nitrogen cooled version available
- Efficient use of cryogen
- Temperature range 1.8 300 K standard (higher temperatures available on request)
- Temperature stability ± 0.1 K

## $Teslatron^H$

Compact high homogeneity Teslatron systems for high field EPR and other applications

- Automated magnetic field and temperature control
- Applied fields from 7 to 20 Tesla
- 10 ppm and 1 ppm homogeneities available
- Integration of experiments using National Instruments LabVIEW®
- Available in ultra low-loss cryostats for greatest cryogen efficiency
- Choice of room temperature access or integral variable temperature insert

Call us now for copies of our Teslatron<sup>H</sup> and ESR product guides

Oxford Instruments
Scientific Research Division
Research Instruments
130A Baker Avenue
Concord, MA 01742 USA
Tel: 1-508-369-9933

Fax: 1-508-369-6616 E-mail: EPR@oxinst.co.uk



transfer dynamics, structural and functional modifications by site-directed mutagenesis.

Over more than three decades he has motivated many colleagues and young scientists from all over the world to collaborate with him in a truly interdisciplinary way to the benefit of science. His impact on the field has been immense and those young scientists who have had extended contacts with him have been stamped by his ambitions and guidelines of scientific standards.

Klaus Möbius Free Univ. Berlin

# Nominations Open for the Zavoisky Award 1997

The Zavoisky Award 1997 will be presented at the annual Workshop "Modern Development of Magnetic Resonance" in September 1997 in Kazan where E. K. Zavoisky demonstrated EPR in 1944. This Workshop is dedicated to the 90th anniversary of E.K. Zavoisky.

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

Nominations are being sought from the EPR community worldwide. A brief presentation of the applicant covering 1-2 pages is expected. The final decision is made by the Award Selection Committee which comprises well-known experts in EPR: B. Bleaney (Oxford), K.H. Hausser (Heidelberg), C.A. Hutchison Jr. (Chicago), Yu.N. Molin (Novosibirsk), A. Schweiger (Zurich) and the Chairman K.M. Salikhov (Kazan).

Nominations should be submitted to Dr. Laila V. Mosina, Executive Secretary of the Zavoisky Award Committee, Kazan Zavoisky Physical-Technical Institute of the Russian Academy of Sciences, Sibirsky trakt, 10/7, Kazan, 420029 Russian Federation. e-mail: mosina@dionis.kfti.kcn.ru. The deadline for submission of nominations is April 1, 1997.

### IES Awards —

All 1998 Nominations are Due by Jan. 1, 1998.

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 among the groups each year, with the three following loosely-interpreted categories: chemistry, physics and instrumentation, and biological sciences (including medicine). These categories are meant to be interpreted very liberally and not to be restrictive.

In 1998, three major awards, the IES Gold Medal, the Bruker Prize, and the Zavoisky Prize will be devoted to the recognition of outstanding achievements in EPR. Prof. Larry Berliner is the continuing Chair of the IES Gold Medal Award Committee.

Gold Medal: Nominations for the 1998 Gold Medal, recognizing benchmark contributions to EPR spectroscopy in Chemistry, should be sent to Prof. Larry Berliner, Chairman of the Gold Medal Committee (e-mail: lberline@magnus.acs.ohio-state.edu) by January 1, 1998.

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 - John Pilbrow, George Feher, and Jan Stankowski. For 'Chemistry- Bruce Gilbert, Chair; N. Hirota, Jim Bolton, and Kev Salikhov. For Biology/Medicine - Harold M. Swartz, Chair; Marjeta Sentjurc, Hideo Utsumi and 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. James R. Norris, Jr.

Fellows of the Society: The IES has created Fellowships to recognize truly outstanding contributions and achievements in electron paramagnetic/spin resonance among distinguished scientists (hopefully, IES members) who are either retired or are close to retirement. (Fellows of 1996: Erwin Hahn, J. H. van der Waals, George Feher). As the highest international standards are to be applied to the recognition of those worthy of this distinction, their formal connection with the Society will enhance its own image. Nominations for consideration by the Committee are to be sent in confidence by January 1, 1998 to Prof. James R. Norris, Jr., Univ. Chicago, Dept. Chemistry - Searle 133,

# NIKKISO Co., Ltd. SUMITOMO SPECIAL METALS Co., Ltd. SUPPORTER of the International EPR Society

Innovative Portable EPR Spectrometer with a built-in 32 bit computer (ES-10)

Frequency: 9.4 Ghz

Sensitivity: 2\*10<sup>10</sup> spins/0.1 mT

Resolution: 6\*10<sup>-5</sup>

Size: 500x500x230 mm

Weight: 25 kg

Magnet: NEOMAX-40



SUMITOMO SPECIAL METALS AMERICA, Inc. (Tel)310-378-7886, (Fax)310-378-0108

Publication of the International EPR(ESR) Society

5735 S. Ellis Ave., Chicago, IL 60637 USA; 3: 1-773-702-7864; FAX: 1-773-702-0805; e-mail: j norris@uchicago.edu.

## THE COMPUTER CORNER

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

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

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

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

\*\*\*\*\*

#### Linux on a PC - Part II

Obtaining the Installation Files and Performing an Installation

by Keith P. Madden

In the last installment of the Computer Corner, we some of the hardware pre-installation considerations for those interested in taking the Linux / GNU operating system for a test drive. This time, we'll explain the installation of a minimal configuration for you to test. Successfully completing this exercise will verify that the Linux kernel will execute properly on your hardware, and provide you with the opportunity to explore this free software UN\*X workalike.

We'll make a few assumptions in the course of this discussion: (1) you have a PC-compatible with a 80386-equivalent or better CPU executing the Intel instruction set - see the last EPR newsletter for further information on hardware aspects / constraints; (2) you have a single large IDE hard drive as your boot drive, formatted as a FAT filesystem, identified as drive C: under DOS or windows, with ~30 megabytes free; (3) you have Internet access to obtain the software we'll be installing, (4) you have ten 1.44 MB 3.5" DOS-formatted, blank floppies available and (5) drive A is your boot floppy drive, a 1.44 MB 3.5" unit. We'll install Linux/GNU on the C: drive in a subdirectory called C:\Linux using a UMSDOS filesystem. UMSDOS uses the FAT filesystem framework of DOS, but extends it in a compatible way to permit the use of both long filenames and the UN\*X scheme of file access control when running under the Linux kernel. We'll install Linux/GNU so that we use a boot disk to start; this will leave the standard boot mechanism unperturbed so that we boot from C: into DOS/Windows as the default choice. Installation of Linux/GNU using a UMSDOS filesystem on a DOS disk

partition is a feature of the Slackware Linux/GNU distribution. We'll obtain the latest Slackware distribution via FTP from the official home of Slackware, the Walnut Creek CD-ROM FTP site ftp.cdrom.com, in their directory /pub/linux/slackware96. We'll use the files that we download to make a set of installation floppies consisting of a boot disk (for booting into Linux / GNU for the installation), a root disk ( containing the package installation program and utilities necessary for decompressing and manipulating the Linux/GNU system files being installed), and a series of eight disks containing the Slackware "A" package. The "A" package contains compressed images of all the programs and configuration files for a base installation. It will be extremely helpful to organize storage for the downloaded files ahead of time, so that we can segregate the files into subdirectories corresponding to the eight "A" series disks. If we make a subdirectory of c:\ named c:\LG FTP, we also create c:\LG FTP\a1, c:\LG FTP\a2, . , c:\LG FTP\a8. We switch to c:\LG FTP as the current directory, and issue the command: ftp ftp.cdrom.com.

An edited transcript of the FTP session follows:

connecting to 165.113.58.253 ...

Connected to 165.113.58.253 port 21

220 wcarchive.cdrom.com FTP server (Version DG-1.0.67 Sun Nov 17 14:47:24 PST 1996) ready.

USER anonymous

331 Guest login ok, send your complete e-mail address as password.

PASS (hidden)

230-Welcome to wearchive - home ftp site for Walnut Creek CDROM.

230-There are currently 684 users out of 1200 possible.

230 Guest login ok, access restrictions apply. PWD 257 "/" is current directory.

CWD pub/linux/slackware96

CWD install

**PWD** 

257 "/.22/linux/slackware-3.1/install" is current directory.

LCD c:\LG FTP

RETR RAWRITE.EXE

**CDUP** 

### RESONANCE INSTRUMENTS, INC. is a CONTRIBUTOR to

The International EPR Society

EPR spectrometers, components, accessories; Model 8320 Magnet Field Controller for Varian's Mark I & II, others, provides keyboard or computer control; microwave instrumentation to 170 GHz.

#### Resonance Instruments, Incorporated

9045 Terminal Drive, Box 1488, Skokie, IL 60077, USA

**☎**: 1-847-583-1000 FAX: 1-847-583-1021

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

CWD bootdsks.144

RETR bare.i

**CDUP** 

CWD rootdsks

RETR umsdos.gz

**CDUP** 

CWD slakware

CWD al

LCD c:\LG FTP\a1

RETR aaa base.tgz

RETR aoutlibs.tgz

RETR bash.tgz

RETR comms.tgz

RETR cpio.tgz

RETR devs.tgz

RETR diskal

RETR etc.tgz

RETR grep.tgz

RETR maketag

RETR maketag.ez

RETR tagfile

RETR tagfile.org

RETR tagfile.pat

**CDUP** 

CWD a2

LCD c:\LG\_FTP\a2

(retrieve the a2 files, continuing the process until all eight a\* subdirectories are full.)

#### BYE

At this point you have all the files needed for installation, but you need to place them appropriately on the floppies. The boot disk file bare.i, and the root disk file umsdos.gz are image files, and need to be copied in a structured manner to their corresponding disks. This is the function of the RAWRITE program. Label one blank formatted disk "BARE BOOT DISK", and insert it in your system's boot drive. Run rawrite, and follow the instructions, loading bare.i to the disk. Do the same for the "UMSDOS ROOT DISK", loading umsdos.gz to the disk (do NOT decompress the file first). Finally label the eight remaining disks A1, A2, A3, ., A8, and copy the files from each "A" subdirectory of c:\LG\_FTP to the appropriate disk using the DOS copy

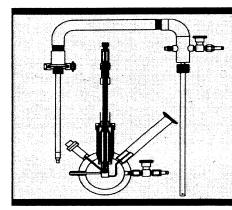
command, i.e. COPY C:\LG\_FTP\A1\\*.\* a: with the A1 floppy in drive a. You will then have the ten disks necessary for your Linux/GNU installation, which we will cover in our next installment.

Why install Linux/GNU?

Under Linux/GNU, the Intel/IBM-compatible has a complete set of UN\*X-compatible networking protocols available to communicate with processes running on remote UN\*X workstations. In addition, the X Free consortium provides XFree86, a free version of X for Intel-architecture PCs, which runs on top of Linux/GNU. X provides distributed computing in the client/server sense, with split responsibility for the execution of a computation-intensive program. The server is the computer serving as the computation engine, typically a capable RISC-based workstation such as the Silicon Graphics Indy, while your desktop PC is the client, providing graphical user interface for data input, graphics rendering, and execution control. This combination will provide an extremely cost-effective, powerful approach to high-performance computing for EPR applications.

Some history of Linux/GNU.

In this, and in subsequent installments of these discussions, I've referred to the Linux operating system as Linux/GNU. This is to make explicit the great contribution of the Free Software Foundation's (FSF) GNU project to the Linux operating system. Almost all of the major utilities in Linux/GNU derive from the efforts of the FSF. The goal of GNU (recursively defined as GNU's Not Un\*x) is to provide low or no-cost access to high-performance computing by developing and distributing freely available, but copyrighted source code and binaries for the UN\*X environment. In our case, the Linux kernel provides the execution environment and the system services for the operating system, while GNU provides the assemblers, compilers, object libraries, debuggers, text editors, and file system utilities to make a functional whole. FSF's copyright of the software preempts the possibility of an individual or organization copyrighting the programs, and making the code proprietary. By owning legally protected, copyrighted code, FSF is able to retain their ability to give it away freely; this is the core of the license



#### **EPR/ENDOR CRYOSTATS**

Complete Systems - Fastest Cooldown - Lowest Temperatures
Uses liquid helium or nitrogen - Push or Pull Operation
Plus, our replacement transfer line for your existing cryostat can Save you up to 50% on your liquid helium costs - Cool down samples faster Lower your terminal temperature and increase reliability!
Call or fax us for additional information:

CRYO Industries of America, Inc. 11 Industrial Way, Atkinson, NH 03811 Tel: (603) 893-2060; Fax: (603) 893-5278

Publication of the International EPR(ESR) Society

agreement between a user and the FSF - affectionately known as the GNU copyleft.

## EPR SPECIALIST VIGNETTES

Edited by Arthur Schweiger

#### **High-Field EPR**

by Thomas F. Prisner
Department of Physics, Free University Berlin
Arnimallee 14, 14195 Berlin
Tel.: 49-30 838 6046 Fax.: 49-30 838 5046
(e-mail prisner@physik.fu-berlin.de)

#### 1. Introduction

Within the last few years a number of spectrometers operating at high magnetic fields and microwave frequencies have been built<sup>1-8</sup>. While a scientific definition of what high field means is strongly system dependent, the terminology high-field / high-frequency EPR is normally used for external magnetic field strengths above 3 T and microwave frequencies above 90 GHz. Technically this is a reasonable choice, because the design of the EPR spectrometer changes at about this frequency. At these high external field strengths, superconducting magnets have to replace the normally used electromagnets and at the corresponding frequencies a transition from classical microwave components and waveguides to far-infrared optical components and quasi-optical beam propagation takes place<sup>1,3,4</sup>. Although technical constraints are still more demanding at such microwave frequencies, several spectroscopic advantages make it worthwhile to undertake the experimental effort.

One of the major goals of high-field EPR is to achieve enhanced spectral resolution. In many cases this is achieved by distinguishing different radicals (or sites in a crystal) by their g values or resolving the powder pattern of disordered systems, caused by their anisotropic g matrix. Where in the first case different species can be spectrally separated and distinguished, sub-ensembles of molecules with a specific orientation (with respect to the external magnetic field) can be selected in the second case. This possibility, to select specific orientations even for disordered systems, offers the opportunity to perform experiments that yield much more detailed information on the anisotropic interactions of the electron spin Hamiltonian. For example ENDOR or ESEEM experiments on such spectrally resolved powder spectra can give the full hyperfine anisotropic information instead of only scalar information<sup>9</sup>. The same holds for relaxation experiments, monitoring the motional dynamics of the molecules10.

For high-spin systems another effect can be of interest: the reduced line broadening of the central transition ( $m_s$ =+1/2 to -1/2) by second-order zero-field splitting at high magnetic fields. In this case a line narrowing is achieved similar to liquid-state NMR applications, allowing for the investigation of other contributions to the linewidth in more detail 11-13

Furthermore, systems with very large zero-field splitting, unobservable at lower magnetic field values, can be investigated at high magnetic fields<sup>14</sup>. Spectra taken at different magnetic field values will facilitate to deconvolute field dependent and field independent parts of the spin Hamiltonian.

Another important aspect of high-field EPR is the strongly enhanced sensitivity of the spectrometer, especially for samples with restricted size as small single crystals. Because of the much higher absolute sensitivity (spins/G) of the spectrometer at higher frequencies, single crystals, much too small to give a signal at usual X-band frequencies, could be observed at high fields<sup>15,16</sup>. It should be kept in mind that this argument doesn't hold for the concentration sensitivity (spins/G/cm<sup>3</sup>) and therefore not for samples that scale with the cavity volume.

## SCIENTIFIC SOFTWARE SERVICES

P.O. Box 406 Normal, IL 61761-0406 USA

Voice/Fax: 309-829-9257

Contributor to the International EPR Society

Cost-effective EPR data acquisition, simulation, deconvolution, and imaging software for ALL EPR spectrometers.

Free DEMOs available.

CALL for further information and pricing
Web site: http://www.wwnet.com/~sss/

Where the increased spectroscopic resolution and the enhanced absolute sensitivity hold for both cw and pulsed EPR applications, there are several additional features making pulsed high-field EPR a specially attractive tool:

Whereas at X-band frequencies the sensitivity of the pulsed experiment is still worse than the sensitivity of the cw experiment for stable radicals, this is no longer true for high-field EPR applications. One of the reasons is that the loaded Q of the cavity at such high frequencies (about 1000 for realistic samples) need not be lowered to perform pulsed experiments, in contrast to experiments at X-band frequencies. Another reason is that the pulsed experiment is much less sensitive to the phase noise of the microwave sources and is not distorted by field modulation microphonics, which are in many cases limiting factors for the sensitivity of cw high-field EPR experiments<sup>13</sup>

At higher microwave frequencies the dimensions of the cavity are decreasing, and therefore the conversion factor of the cavity (excitation power to rotating microwave field  $B_1$ ) is increasing. The combination of larger cavity bandwidth and smaller necessary microwave excitation power leads to a very short dead time of the spectrometer. Unfortunately, because of technical reasons, the pulse lengths are rather long (30-100 ns), limiting the achievable time resolution.

In principle, all the pulsed EPR methods developed at X-band frequencies can also be used at high frequencies to further increase spectral resolution, manipulate and observe

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

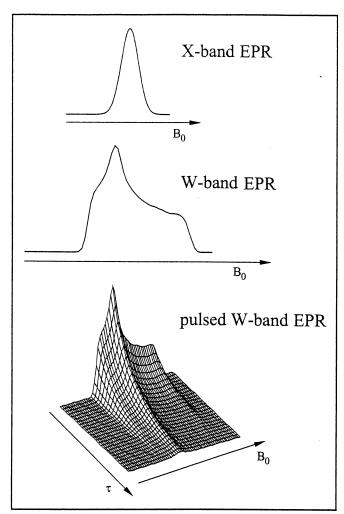


Figure 1: Spectral resolution, sketched on a ubiquinone anion radical. The enhanced resolution from X-band EPR spectra to W-band EPR spectra and to a 2-D W-band 2-pulse echo decay experiment are illustrated.

nuclear coherences, generate and detect multi-quantum coherences for example. Additional gain in information for disordered systems can be obtained at high fields by performing the pulsed experiments on spectrally resolved sub-ensembles of molecules, representing specific orientations. In this case, orientational anisotropies of relaxation effects can be resolved. In many cases, these orientational anisotropies may allow one to draw more direct

## JEOL USA, Inc.

Manufacturer of CW Electron Spin Resonance Spectrometers Featuring a Compact Design with High Sensitivity and High Reliability

11 Dearborn Road, Peabody, MA 01960, USA Phone: 1-508-535-5900; FAX: 1-508-536-2205 E-mail: dipas@jeol.com conclusions than the absolute values of the relaxation rates do. Furthermore high-field EPR has an increased sensitivity for monitoring motional dynamics<sup>17,10</sup>. Measurements of the relaxation dynamics at different magnetic field values will allow to distinguish the responsible physical process by its field dependence.

The combined advantages of increased spectral and time resolution is sketched in Figure 1. There a ubiquinone radical spectrum is shown at X-band (top) and W-band (middle) frequencies, demonstrating the ability to resolve the anisotropic g-matrix at high frequencies, where at X-band frequencies the spectrum is dominated by unresolved hyperfine coupling. The spectral resolution can still be increased by performing pulsed experiments (bottom), in this case orientation-dependent anisotropies in the homogeneous linewidth can be resolved, unobservable even in the high-field cw-EPR spectrum.

ENDOR experiments performed at high fields are a very powerful tool. Again they profit from the spectral resolution obtained in the EPR spectral dimension. Additionally the spectral resolution in the nuclear frequency dimension is strongly increased, separating hyperfine couplings from different nuclei (<sup>13</sup>C, <sup>14</sup>N, <sup>15</sup>N, <sup>17</sup>O, <sup>31</sup>P, <sup>1</sup>H, <sup>2</sup>H) by their different Zeeman splittings. For many nuclei the high-field approximation is valid; therefore spectra are further simplified.

#### 2. Instrumentation

Classical microwave devices are available up to frequencies of about 150 GHz. Above that frequency far-infrared optical components or microwave tube devices, quasioptical transmission lines and hot electron bolometers are used, differing more strongly from the common X-band EPR spectrometer design. The design of high-field EPR spectrometers is strongly dependent on the major field of application they are used for:

For typical solid-state physics systems with broad lines, an extremely large sweep range is often necessary. In this case the main coil of the magnet has to be swept, which leads to a poor field homogeneity, linearity and absolute accuracy. If the spectrometer has to be able to work at different microwave frequencies, broadbanded microwave sources, transmission lines and detectors are used. This broadband design leads to a strongly reduced sensitivity of the spectrometer.

For many organic molecules in chemical and biochemical applications only a small magnetic-field sweep range is needed, but requirements on field homogeneity, sweep linearity and absolute field calibration are much more demanding. In this case an additional sweep coil facilitates performance and accuracy. For this applications sensitivity is of major concern, therefore phase-locked narrow-banded sources, tuned cavities and detectors with low noise figures have to be used. Performance of active devices are far from ideal at these high microwave frequencies and not always even adequately specified. The noise behaviour of the microwave sources are problematic, specifically for cw applications, where the noise is probed some KHz offset

Publication of the International EPR(ESR) Society

from the carrier only. Cavities with high Q values and under matching conditions have to be used to get maximum sensitivity. Because optimal sensitivity is mandatory for diluted spin systems, no compromise can be made with respect to the performance of the cavity. Therefore selection of sample size, solvent, and positioning of the sample inside the cavity has to be done very carefully. Microwave losses of the samples are often stringent at high microwave frequencies; thus very small sample capillaries or cells have to be used. For example, water samples in our cylindrical cavity (TE<sub>011</sub> mode, 95 GHz, room temperature) have to be smaller than 0.2 mm in diameter. This makes sample preparation, degassing and handling troublesome. The sample not only degrades the Q of the cavity, but also leads to a mismatch of the cavity and thus to reflected microwave power. Because of the circular symmetry of the Fabry-Perot resonator, degradation of the spectrometer sensitivity by reflected microwave power can be strongly suppressed by using the orthogonal mode for the detection of the signal. This is also necessary for pulsed experiments with high power microwave sources to protect the sensitive microwave mixer. A suppression of 40 dB of the excitation pulses was measured with such a bimodal configuration at 140 GHz<sup>18</sup>. At higher microwave frequencies, where ferrite circulators are not available, this scheme can be used for duplexing between excitation and detection branch.

In the detection channel the noise figure of preamplifiers, mixers and detectors is much worse than what is standard at X-band frequencies; nevertheless, because of the higher microwave frequency, the absolute sensitivity can, in ideal cases, still be orders of magnitudes better.

#### 3. Applications

There are rather diverse fields of applications of high-field EPR, as already mentioned above. One important class of applications are transient or stable paramagnetic centers in biological systems. In many cases, their g factors differ only a tiny little bit, and their respective g anisotropies are also much smaller than other inhomogeneous broadening contributions to the linewidth. Therefore high magnetic fields are necessary to get them separated and to achieve spectral resolution of the g matrix anisotropy. This can be used to get orientational selection even on these normally disordered systems. Some examples out of our recent work will be given in the following for illustration.

The g anisotropy of the quinone anion radical is nicely resolved at 3.4 T magnetic field (Figure 1 middle). Therefore orientation-selective experiments (Echo decay function and ENDOR) could be performed on this radical. In Figure 1 (bottom) the two-pulse echo decay as a function of the magnetic field is shown. The strong anisotropy of the echo decay function with respect to the magnetic-field position can be used to investigate the librational motion of the molecule in very detail 10. This information cannot be obtained at X-band frequencies because the g anisotropy is not resolved at 0.3 T and additionally the influence of the librational motion on the echo decay is strongly reduced.

Figure 2 shows the spin polarized 95 GHz EPR spectrum

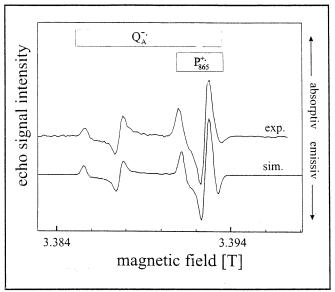


Figure 2: Spin-polarized spectrum of the transient correlated radical pair P<sup>+</sup>-Q<sup>-</sup> of bacterial reaction centers R-26. The spectral range of the two radicals is indicated on top of the spectra. The simulation determines the relative orientation of the two respective g-matrix axis systems with respect to the dipolar axis.

of a transient radical pair in a Zn-substituted bacterial reaction center of *rhodobacter sphaeroides* R-26, created by a fast electron transfer reaction after flash photoexcitation. The spectral components of the two radicals (an ubiquinone anion and a chlorophyll dimer cation radical) are partly separated at high fields, as indicated in Figure 2. Therefore detailed information on the relative orientation of the two molecules in the protein could be obtained<sup>19</sup>.

An example for the line narrowing for the central transition ( $m_s = +1/2$  to -1/2) for high-spin systems at high magnetic field is shown in Figure 3. One hyperfine line (m<sub>1</sub>= - 5/2) of a Mn<sup>2+</sup> center for 3 different p21 ras GDP protein complex preparations is shown. The native system shows a much narrower line at high magnetic field values. This is because the linewidth contribution from second-order zerofield splitting is scaled down proportional to the magnetic field. Therefore hfi contributions from coupling of the Mn<sup>2+</sup> center to other nuclei can be observed more easily. In Figure 3 such <sup>17</sup>O hyperfine couplings are resolved for a sample with a specifically labeled oxygen at the  $\beta$ -phosphor position of the GDP complex (middle spectrum) and for a sample in H<sub>2</sub><sup>17</sup>O (outer spectrum). Therefore hyperfine coupling constants, water coordination number, and therefore also the binding of the metal to the protein can be investigated with high accuracy  $^{11,13}$ .

#### 4. Summary and Outlook

Several applications have proven the use of high-field EPR in rather diverse fields. The increased information content of high-field EPR in one special field of applications, namely organic radicals in disordered biological samples, has been sketched here. In this case, the information content of spectra taken at X-band frequencies is often too low to assign unambiguously all the parameters (often even tensorial) of the spin Hamiltonian. High-field EPR and ENDOR can help

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

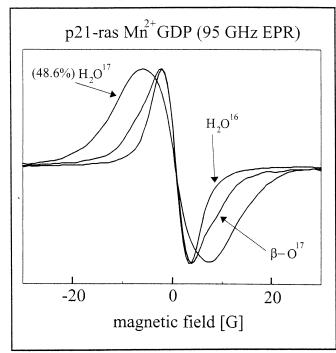


Figure 3: High-field EPR spectra for 3 different protein preparations: the native system (narrow line), GDP specifically labeled at the  $\beta$ -position by  $^{17}{\rm O}$  (medium line) and protein in  ${\rm H_2}^{17}{\rm O}$  (48.6%) (broad line), shown is only the line  $m_I$ =-5/2 Mn-hyperfine line of the  $m_S$ =-1/2+1/2 transition. The measurements are performed at room temperature with only 10 nl of sample (10 $^{-3}$ mol/l).

in these cases to unravel the anisotropies and therefore the matrix or tensor character of the different interactions. This doesn't mean that the low-frequency experiments are not necessary for these samples. Instead, multi-frequency experiments performed at different external magnetic field strengths help to separate the different contributions by their specific field dependence and consolidate assignments done at one microwave frequency. Which frequency is the optimum frequency cannot be answered generally. Limitations to higher frequencies and magnetic field strengths are more of technical nature. For experiments where a high magnetic-field homogeneity is required, superconducting magnets have to be used. This sets an upper limit of 500 GHz to the microwave frequency (for g=2 systems). Classical semiconductor devices have their upper border at about 150 GHz. Microwave tube devices extend the frequency range up to 1 THz, but are rather costly, mostly because no commercial application above 100 GHz exists. Infrared technology develops its full beauty above 1 THz, but may be used down to 100 GHz. Sample handling and sample losses may also limit the usable frequency. Nevertheless there is a growing interest in high-frequency EPR. At 95 GHz there is already a commercial spectrometer available, and several research groups are at the moment developing the potential of sub-mm EPR, above 300 GHz.

#### REFERENCES

- K. A. Earle, D. S. Tipikin, J. H. Freed, Rev. Sci. Instrum. 67, 2502 (1996).
- 2. Ya. S. Lebedev, Appl. Magn. Reson. 7, 339 (1994).
- A. L. Barra, L. C. Brunel, J. B. Robert, Chem. Phys. Lett. 165, 107 (1990).
- C. Kutter, H. P. Moll, J. van Tol, H. Zuckermann, J. C. Maan, P. Wyder, Phys. Rev. Lett. 74, 2925 (1995).
- J. A. J. M. Disselhorst, H. van der Meer, O. G. Poluektov, J. Schmidt, Journ. Magn. Reson. A115, 183 (1995).
- L. R. Becerra, G. J. Gerfen, B. F. Bellew, J. A. Bryant, D. Hall, S. J. Inati, R. T. Weber, S. Un, T. F. Prisner, A. E. McDermott, K. W. Fishbein, K. E. Kreischer, R. J. Temkin, D. J. Singel, R. G. Griffin, Journ. Magn. Reson. A117, 28 (1995).
- T. F. Prisner, M. Rohrer, K. Möbius, Appl. Magn. Reson. 7, 167 (1994).
- W. Wang, R. L. Belford, R. B. Clarkson, P. H. Davis, J. Forrer, M. J. Nilges, M. D. Timken, T. Walczak, M. C. Thurnauer, J. R. Norris, A. L. Morris, Y. Zhang, Appl. Magn. Reson. 6, 195 (1994).
- M. Rohrer, M. Plato, F. MacMillan, Y. Grishin, W. Lubitz, K. Möbius, Journ. Magn. Reson. A116, 59 (1995).
- M. Rohrer, P. Gast, K. Möbius, T. Prisner, Chem. Phys. Lett. 259, 523 (1996).
- 11. B. F. Bellew, C. J. Halkides, G. J. Gerfen, R. G. Griffin, D. Singel, Biochemistry 35, 12186 (1996).
- 12. M. Geyer, T. Schweins, C. Herrmann, T. Prisner, A. Wittinghofer, H. R. Kalbitzer, Biochemistry **35**, 10308 (1996).
- 13. T. F. Prisner, Advances in Magnetic and Optical Resonance, Vol. 20, ed. W. W. Warren, (in press).
- 14. A. Dei, D. Gatteschi, L. Pardi, A. L. Barra, L. C. Brunel, Chem. Phys. Lett. **175**, 589 (1990).
- E. J. J. Groenen, O. G. Poluektov, M. Matsushita, J. Schmidt, J. H. van der Waals, G. Meijer, Chem. Phys. Lett. 197, 314 (1992).
- 16. R. Klette, J. T. Törring, M. Plato, K. Möbius, B. Bönigk, W. Lubitz, Journ. Phys. Chem. 97, 2015 (1993).

# Summit Technology Inc.

8827 Osceola Ave. Morton Grove, IL 60053

Phone: 1-800-735-6327 / 1-847-470-1638

Fax: 1-847-470-1562

Email: 73173.1415@compuserve.com

http://ourworld.compuserve.com/homepages/summit1

## Supporter of the International EPR(ESR) Society

- **♦**EPR Spectrometers
- ♦ Microwave Bridges
- ◆Magnetic Field Controllers
- ♦ Variable Temperature Controllers
- ◆Spectrometer Repair and Modification
- ♦ Visit our home page on the world wide web

Publication of the International EPR(ESR) Society

- 17. D. Budil, K. Earle, W. B. Lynch, J. H. Freed *Advanced EPR*, Ch. 8, edit. A. J. Hoff, Elsevier, Amsterdam (1989).
- T. F. Prisner, S. Un, R. G. Griffin, Isr. Journ. Chem. 32, 357 (1992).
- 19. T. F. Prisner, A. van der Est, R. Bittl, D. Stehlik, W. Lubitz, K. Möbius, Chem. Phys. 194, 361 (1995).

## Building the Perfect Beast

by Chris Bender NIH Biotechnology Resource for Pulsed EPR bender@spin.aecom.yu.edu

This issue's topic has a moralistic story that accompanies a humbling experience. A while back I was in the throes of rerouting semirigid coax all around our lab, and I decided to buy an Omni-Spectra assembly kit for putting every imaginable type of SMA connector on every imaginable dimension of semirigid coax. I decided that any gadget that had the potential of making my life easier deserved to be bought. I imagined precise connections, lower losses (i.e. VSWR) in my circuits, and the end of those endless adjustments as I misjudge the proper length to cut (dielectric, outer shield, inner conductor). The kit arrived in a very nice wooden box, and I admired the shiny little gadgets. Unfortunately the manual shows only close-up sketches of the things 'in action'; I couldn't figure out how to set up the jigs. I'm also embarrassed to say that the way I was using the devices was akin to the scenario that occurs when you buy your kid an erector set, and he goes off and plays with the box.

Last weekend, when no one was around, I once again took out the Omni-Spectra kit (in its still shiny pristine

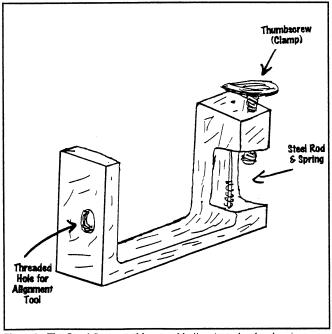


Figure 1. The Omni-Spectra cable assembly jig. A steel rod and spring serve to align and provide tension in the wooden black 'clamp' (see Figure 2 for assembly details). Thumbscrew locks the wooden block halves together around the cable section.

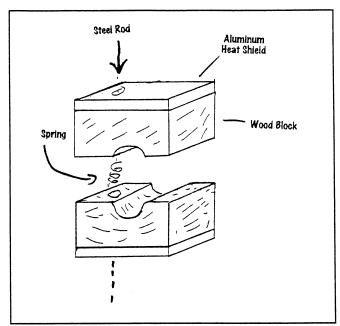


Figure 2: The wooden block clamp for holding cable section. The spring is removed from the jig/steel rod and nested in a well between the two blocks (wood side facing in). The steel rod is passed through the wood blocks and spring, then inserted in the cutout in the jig. The thumbscrew is used to apply pressure for closing and locking the wooden block clamp.

wooden box) and did battle with it. I am happy to report that I conquered it and decided that, in case there are others of you who have sheepishly put a similar kit in a dark forgotten place, I'd reveal the secrets of the Omni-Spectra test jig.

The jig is a steel C-frame that has a screw-threaded hole on one side and a weird looking device that resembles a thumbscrew in the other (Figure 1). There are also pairs of little blocks that have a metallic face and a wooden face. Besides the thumbscrew, there is a removable rod on which is a small spring.

Once the device is assembled, the manual and its line drawings make perfect sense. The wooden blocks are intended as a clamp for the semirigid guide during alignment and soldering; the wood acts as an insulator when you are heating the cable jacket. They are inserted onto a shaft under spring-loaded tension, and the 'thumb-screw' is used to lock the blocks in place around the coax cable. The steps of assembly are illustrated in Figure 2.

Opposite the now-assembled clamps, there is a threaded hole in the vertical portion of the frame. This is where a depth gauge and alignment tool is inserted. The alignment tool is screwed in place, and the clamped coax cable is threaded through the opening in the wooden blocks so that the cable end and alignment tool abut.

## INTRIGUING (and BEGUILING) OSCILLOSCOPE DISPLAYS

When I first started this series of articles I listed many reference books and mentioned the MIT Radiation Laboratory Series. I also made a remark that certain volumes, specifically naming the CRT book, were obsolete and bordering on useless. I was browsing that CRT book the

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

## 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

other day, and found a rather neat little technique that I found potentially useful (or at least entertaining) for pulsed EPR.

It's possible to set up a circular sweep pattern on the CRT/scope. Basically, what you do is drive the two orthogonal pairs of deflector plates with sinusoidal waveforms that are offset in phase by 90°. A rough sketch of the driver circuit is depicted in Figure 3. The technique was originally used to check the stability of pulse/frequency generators; if the pulse is occurring at a stable rep rate, the 'pip' stays put at some position along the circular trace (Figure 4).

If one is familiar with Lissajous figures and how to generate them on the older x-y oscilloscopes, one can easily set up a type of circular display in order to demonstrate the principles; the actual circular display mode is just a little bit more involved due to phase and amplitude tweaking. The application that came to mind, however, is that the circular display is actually an improvement over the linear display that I use to track my pulses and set up the timing parameters of the pulsed EPR spectrometer. For one thing, it roughly trebles the time span covered in a single sweep (you're working with a circumference, which goes as  $\pi d$ , d being your linear sweep length). The display also gives you a clock-like monitor of the microwave pulses (and echo, if you set up

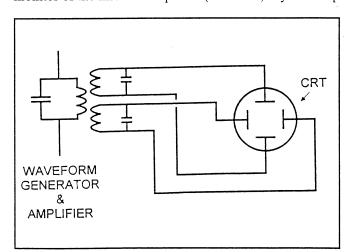


Figure 3. CRT driver for circular traces. A waveform generator supplies input to a resonant circuit element that is tapped by a transformer pair. The two transformer circuits are tuned so that their waveforms are 90° out of phase.

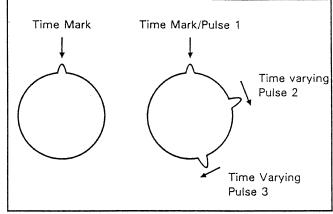


Figure 4. Rendition of the circular oscillograph and application. As a time/frequency test instrument, the pulse will appear stationary (left) if the pulse frequency coincides with the rate of the circular sweep. As a monitor for a pulsed EPR experiment, the pulses would race around the circular path as tau (two pulse) or 5 (three pulse) was varied.

a monitor for it). The stationary pulses will persist at the same locale along the circle, while the time-variant pulse will run around the perimeter as the system scans. If you take the trouble to synchronize step size, sample rate, etc. you can get the time variant pulse to complete one revolution in a scan.

Greenwood, I.A.; Holdam, J.V.; Macrae, D. 1948. Electronic Instruments, *MIT Radiation Laboratory Series Volume 21*, McGraw-Hill: New York.

## TIPS & TECHNIQUES

A SIMPLE DEVICE FOR THE PRECISE POSITIONING OF A LINE-LIKE SAMPLE IN THE RECTANGULAR CAVITY.

Milan Mazur and Harry Morris\*

Department of Physical Chemistry
Faculty of Chemical Technology
Slovak Technical University
Radlinskeho 9, SK-812 3 7 Bratislava, Slovakia
E-mail: mazur@cvt.stuba.sk

\*School of Pharmacy and Chemistry Liverpool John Moores University, Byrom Street, Liverpool L3 3AF UK

Previous studies have shown that sample size, shape and positioning within the microwave cavity result in a nonuniformity of both the microwave and modulation fields [1-6] thereby introducing significant errors in quantitative EPR spectroscopy.

The aim of this technical note is to suggest methods for minimisation of the above sources of error by means of a simple procedure for the insertion of the reference and unknown samples in the TE<sub>102</sub> single rectangular cavity. This technique minimises both the microwave and modulation field perturbation whilst still giving an acceptable

Publication of the International EPR(ESR) Society

signal/noise ratio. The procedure is sufficiently simple for routine quantitative experiments.

Most methods of holding the sample within the cavity involve using commercially available holders, usually delivered with the EPR spectrometer. A simple procedure for quantitative EPR measurements using a cylindrical ( $\approx 3$  mm o/d.) full-length cavity sample tube was developed by Chang [7] and an arrangement for measuring the intensity of a point-like sample, e.g. a crystal about 0.1 mm in size, was discussed by Nagy and Plaček [4]. The method described herein is an extension of both these methods applied to a TE $_{102}$  single rectangular cavity and aims to achieve sample positioning within the cavity as close as possible to the ideal position.

A schematic diagram of the setup for application with the  ${\rm TE}_{102}$  cavity is shown in Figure 1.

The rectangular cavity (A), waveguide to the microwave bridge (C), sample access hole (D) and the iris (T) are all part of the standard cavity as supplied by the manufacturer. The point (P) is the centre of the cavity. The thin-walled quartz tube (E) can be of variable diameter (e.g. 4 mm o/d.), is fixed to the cavity, and acts as a centring/alignment guide for the remainder of the sample assembly. This consists of a rod (F) with a calibrated micrometer screw and holder (G) to which the EPR sample tube (J), (variable diameter, e.g. 1.5 mm o/d., 60 mm length) is attached via the connector (K). The teflon 'O' rings (I) are attached to the sample assembly and ensure that the sample tube (N) is concentric with the axis of the fixed quartz tube (E). The marker (M) is the upper filling position for the sample of length L and marker (R) is for calibration.  $\Delta x$  represents the vertical freedom of movement of the sample with respect to the central cavity axis. Stopper and marker (H) allows realignment of the sample during removal and reinsertion of the sample. Parts (F-S) form the sample assembly which is inserted or removed in its entirety with the sample. Parts (I, J, K) are changed only when the o/d. of the sample tube is changed, and part (E) needs only to be changed if the o/d. of the sample tube is in excess of 3mm. Sample length (L) can be varied from 1 mm (point-like sample) to 50 mm (line-like sample); however, wherever possible L should be equal to L' (length of reference sample) although experience has shown that acceptable results can be obtained where this is not the case.

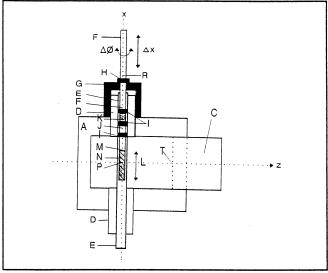


Figure 1. Schematic diagram of the cross section of the  $TE_{102}$  single rectangular cavity with the modified sample arrangement for quantitative EPR measurements.

The quartz tube (E) is permanently fixed to the cavity and centred along the x-axis using cavity-excess-hole-plugs (D). When the sample assembly is inserted, the 'O' rings accurately fix the lateral position but allow variation in the vertical position through the centre of the cavity (P). The vertical position of the sample within the cavity can be varied by rotating a calibrated micrometer screw on rod (F) into the matrix screw (G), enabling accurate positioning of the sample within the cavity to better than 0.1 mm; thus, signal peak-to-peak intensities can be studied as a function of position,  $\Delta x$ . The final, optimal, sample position is marked using the stopper/marker (H).

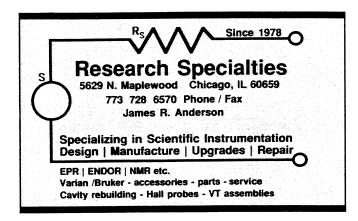
Reinsertion and/or changing the sample tube is achieved by removal of the entire sample assembly vertically out of the cavity, disconnection of the current sample tube at joint (K), replacement of the sample tube with one of the same size, transfer of the 'O' rings and reinsertion in the cavity at exactly the same position as the original using the stopper (H). The procedure is simple, accurate, fast and routine and the only additional component from the assembly within the microwave field is a small teflon 'O' ring (about 1 mm wide), which has a negligible perturbative effect. Thus the

## **GMW** Associates

- Laboratory Electromagnets & Power Supplies
- Precision Hall Effect Teslameters
- Digital NMR Teslameters
- Digital Voltage Integrators
- Precision Current Transducers

Specializing in Magnetic Measurements and Electromagnet Systems
PO Box 2578, Redwood City, CA 94064 USA. Tel (415)802-8292 Fax (415) 802-8298

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA



assembly itself introduces no additional sources of error whilst allowing known sources of error to be minimised.

The size and shape of the actual sample and reference tubes are identical and can be precisely positioned within the cavity; thus the remaining variable parameters are the instrumental factors associated with the retuning of the cavity and the actual size of the sample. The latter is limited by two opposing factors: (i) minimising field perturbations (optimised by as small a sample as possible) and (ii) maximising the signal/noise ratio (in principle by as large a sample as possible). A suitable compromise was found with a cylindrical sample 1.3 mm i.d., as compared to the usual sample tube diameter of about 4 mm i.d. This gives a filling factor of approximately ten times less, with consequent reductions in the microwave and modulation field perturbations, whilst still giving an acceptable signal/noise ratio. In practice the amount of sample is measured in terms of the length of the sample rather than by volume and the reproducibility is enhanced using sample tubes with a standard length marker, although care still has to be exercised to ensure that, in the case of solid powdered samples, the packing density is constant. With these procedures, the EPR signal intensity of identical full-length cavity line-like samples which were packed by the same procedure with the same powdered material into identical sample tubes could be measured using the same instrumental parameters to a precision of between 3-5 %; however, if no additional precautions were taken then errors could be over 20%.

In conclusion, using a simple modification to the sample insertion procedure for the Bruker  ${\rm TE}_{102}$  cavity described above leads to a significant increase in the accuracy to which quantitative EPR measurements can be made. The adaptation can be used with the double  ${\rm TE}_{104}$  cavity without modification (see ref [8]), and with the cylindrical (e.g.  ${\rm TE}_{O11}$ ) and other manufacturer (e.g. Varian) cavities with minor modifications. A detailed analysis of errors associated with quantitative EPR measurements is given in ref [9].

#### REFERENCES

- C. P. Poole, Electron spin resonance. A comprehensive treatise on experimental techniques, Wiley-Interscience, New York, 1967.
- 2. G. Casteleijn, J.J. ten Bosch and J.J. Smidt, Appl. Phys., 39 (1968) 4375.

- D.P. Dalal, S.S. Eaton and G.R. Eaton, J. Magn. Reson., 44 (1981) 415.
- 4. V.J. Nagy and J. Plaćek, Fresenius J. Anal. Chem., 343 (1992)
- 5. R.C. Barklie and L. Sealy, J. Magn. Reson., 97 (1992) 611.
- M. Sueki, G.A. Rinard, S.S. Eaton and G.R. Eaton, J. Magn. Reson, Serie A, 118 (1996) 173.
- 7. R. Chang, Anal. Chem., 46 (1974) 1360.
- 8. M. Mazur, M. Valko, R. Klement and H Morris, Anal. Chim. Acta, 333 (1996) 249.
- M. Mazur, M. Valko, H. Morris and R. Klement, Anal. Chim. Acta, 333 (1996) 253.

## **LETTERS**

#### OPEN LETTER FROM DAVID GREENSLADE

Dear Friends and Colleagues:

In 1982, the Nuffield Foundation, a U.K. Charity founded by Lord Nuffield of Morris and MG Car fame, gave me a grant to visit the U.S. to study the construction and use of pulse e.s.r. spectrometers. Although there had been some work in the Clarendon Laboratory in Oxford, this area seemed to be neglected in the U.K. and thus qualified for support from a scheme of that foundation, which aimed to help U.K. scientists learn new techniques. I made flying visits to a number of laboratories, starting with Bell Labs, where Bill Mims made me feel at home not only by his helpful advice, but also by speaking in an English accent. But native born Americans were also most helpful, and our current president, Jim Norris offered much help, including the offer of software should I use the computer and pulse programmer used at the Argonne Laboratory. Unfortunately, on returning to the U.K., I encountered, when I and a number of colleagues applied to our science research council, a negative and ill informed attitude in the U.K. chemical community. One referee of our grant application asked why we wanted an expensive Nicolet computer, when DEC Corporation could supply one for much less than the figure in our grant - he had not read the line in the application that pointed out the cost included a pulse programmer interfaced to the computer and the above mentioned offer of software to drive the experiment! In the event one of my senior colleagues withdrew from the



Publication of the International EPR(ESR) Society

## WILMAD GLASS Co.

## is a CONTRIBUTOR to the International EPR Society

"Serving the Spectroscopic Aftermarket"

EPR Glassware/Quartzware. Sample cells. Dewars.

Address: Route 40 & Oak Rd. Buena, NJ 08310, USA

609-697-3000 / 609-697-0536 Phone/FAX:

programme, with the comment that we would "never get past

that sort of refereeing". I think he should have added " or that sort of committee and secretariat that allows it". In the event all was not lost as the Engineering Board of the U.K. Science and Engineering Council did give me support on the basis that a commercial instrument was not then available and the equipment might be of industrial importance ( can anyone give me an example or were they mistaken). The committee concerned did not, however have great funds, and so I was asked to investigate a way of making a low cost instrument. As a result we looked at magnetrons as these were used in the early spectrometers. In fact near here at Chelmsford is the headquarters of the EEV company and a number of their staff have been most helpful over the years. They suggested the pedestal pulse phase priming method for coherent pulses, and over the next few years we developed this obtaining a U.K. patent eventually. The method does have problems: no commercial pulse power supply is available, I believe, suitable for this method, which uses a two stage voltage pulse to drive the magnetron into oscillation. Also the magnetron oscillates at a different frequency from the phase priming signal (which in our case was about 100 mW from a Ferranti crystal oscillator/multiplier unit) and so second detection of the intermediate frequency is needed. The advantage of cheapness - our MG5248 marine magnetron costs a mere 100 G.B. pounds - is offset by a fixed frequency. We had to build a tuneable cavity, although Dr Keith Sales, of Queen Mary and Westfield College in London University later gave me their redundant variable frequency Decca cavity. Of course, Varian did make a more expensive variable frequency magnetron. Only one Decca c.w. ESR instrument was exported form the U.K., I believe, and that to Israel, so anyone outside the U.K. wishing to follow our work has to make their own cavity! We found making a modulator, or pulse generator stretched our electronic expertise and the design I produced suffered from transistor breakdown, although with the help of Mr. Harry Kitchin of Bournlea Instruments, Bentley Manor, Ipswich, we did get some stimulated echo results. Prior to that we had modified a Mars Electronics, small boat RADAR transmitter to show the principle over short time intervals/pulse spacing. As Jim Norris pointed out to me some time ago, solid state amplifiers can replace TWTA's - of course, they tend to be of lower bandwidth. This is not so bad as most people do not operate their spectrometers either wideband or full power. So we bought a Pascall 25 watt amplifier and have used this to do stimulated echo work. Like

the TWTA it emits quite a lot of noise despite being of only 500 MHz bandwidth, so that a switch is needed after it to cut out the noise. I decided that the simplest approach to pulse programming when we started ten years ago, was to use the CAMAC system so familiar in nuclear physics and also processs control. I use a LeCroy unit with one of their IEE488 crate controllers driven from a Ferranti 286AT computer fitted with an IEE488 interface card. The crate contains a LeCroy 4222 timing unit (four channels at one nanosecond resolution), a gated integrator from Evans (of California) - another JRN suggestion - and homebuilt pulsewidth modules based on monostable circuits. It seems a pity that all this work is now being laid to rest: the shortage of students, cash and political expediency has resulted in such a bad atmosphere here at the University of Essex that I am taking early retirement and it looks, since no other institution is able to offer me a home, as if the equipment is to be scrapped! I will be happy to talk to anyone who wants to build a low-cost pulse EPR: perhaps I may add "have hands and brain will travel!" Many thanks to all those scientists who have helped by talking and listening to me!

> David Greenslade E-mail: greed@essex.ac.uk 6, St. Faith Road, Colchester CO4 4PS, UK Telephone +44 (international) or 0 - 1206 84 32 84

## **COMPANY PROFILES**

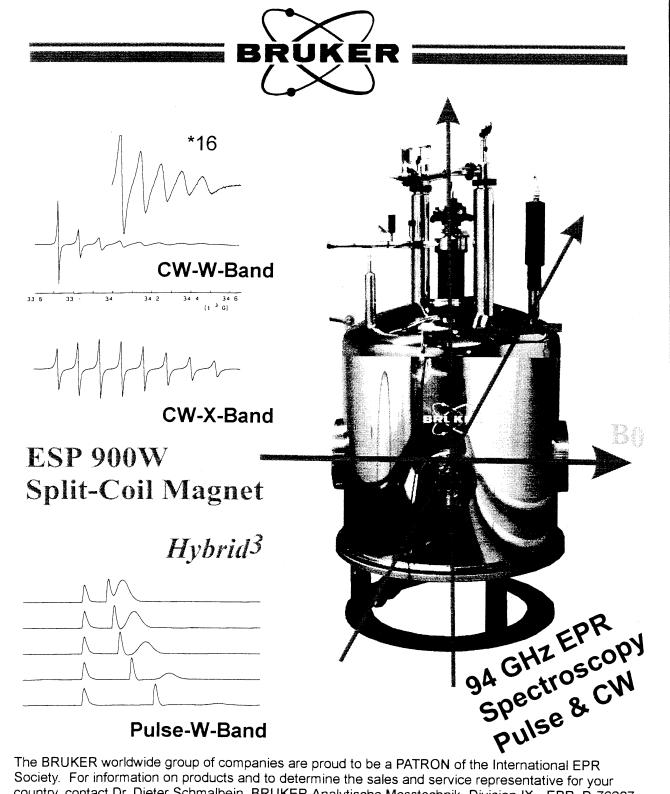
## Scientific Software Services

Scientific Software Services started in 1988 with the goal of providing data-acquisition software and hardware for EPR spectroscopy with its EW data acquisition package. Since that time, the company has expanded its product line to include simulation and deconvolution software, EPR imaging, and ENDOR.

Recent additions include: 1) EWVOIGT, a spectral deconvolution/simulation program for imhomogeneously broadened EPR spectra which calculates Gaussian and Lorentzian linewidths and 2) a complete EPR imaging laboratory for teaching the principles of imaging at the level of introductory Physical Chemistry.

With over 130 systems in operation all over the world, Scientific Software Services is the largest company dedicated solely to EPR-application software. Installations have been performed on Bruker, JEOL, MicroNow (now Resonance Instruments), and Varian EPR spectrometers. Our imaging product helps NASA detect defects in polymers and teaches students the principles of magnetic resonance imaging at the University of Illinois and Illinois State University.

To date, the product lines offered have been based on PC's running DOS. However, improvements in computer power and drastic decreases in price (32 megabytes of computer memory can now be purchased for under \$150.00) have made the desktop PC amenable to more graphically-oriented operating systems such as Windows and UNIX/



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: 49-721-51 61-141; FAX: 49-721-51 61-237; email: epr\_sales@bruker.de. In the USA, contact Dr. Arthur Heiss, BRUKER Instruments, Inc., 19 Fortune Drive, Manning Park, Billerica, MA 01821. Telephone: 508-663-7406; FAX: 508-670-8851; email: ahh@bruker.com.

PAID ADVERTISEMENT

Publication of the International EPR(ESR) Society

Linux/XWindows. Also, the rise of strictly UNIX machines (exemplified by Sun Microsystems, Silicon Graphics, and Digital Equipment Corporation) and the increased power of the Macintosh (a 533 MHz CPU is under development for the Mac) make these computers attractive for EPR applications.

To take advantage of the growing computational power, Services Software has developed platform-independent EPR data-acquisition package which is currently undergoing testing. The hardware is a dataacquisition card controlled by a stand-alone single-board computer with all program and data in a battery-backed RAM module (no data loss upon power loss). Communication with the processing computer is through a high-speed serial line (EtherNet and parallel-port versions are under development), which means that the user is no longer tied to a given computer type. The software which drives the data-acquisition module currently runs under Microsoft Windows (it has been run under Windows 3.1, 3.11, NT, and 95), but could be ported to any computer running any common operating system.

We want this system to meet the needs of the EPR community and so we are asking for your help in testing and evaluation. Please send comments, suggestions, questions, and ideas to Scientific Software Services at sss@wwnet.com. We welcome your contributions and, although they will become the property of Scientific Software Services, we will acknowledge your contributions both in the user manual and in the "About..." box.

You can download the demonstration version of EWWIN (for a PC) from http://www.wwnet.com/~sss/ as three separate files which will self-extract into the entire software package and the user manual. The data-acquisition portion of the software is simulated, but performs essentially as it would in the complete package.

In the near future, we will be porting our DOS simulation and spectral deconvolution software (EWSIM and EWVOIGT) to Windows (and other platforms), so your comments will go a long way toward deciding the shape of Scientific Software Services' products in the years to come.

For more information contact Scientific Software Services, P.O. Box 406, Normal, IL 61761-0406, USA; **\$\infty\$**/FAX: 1-309-829-9257; Website: http://www.wwnet..com/~sss/.

## **NOTICES OF MEETINGS**

NATO ADVANCED WORKSHOP, "MOLECULAR MODELING AND DYNAMICS of BIOLOGICAL MOLECULES CONTAINING METAL IONS," March 15-21, 1997, San Miniato, Pisa, Italy.

For further information please contact: Prof. Lucia Banci, Univ. Florence, via Gino Capponi 7, 50121 Florence, Italy; **2**: 39-55-2757550; FAX: 39-5-2757555;

E-mail: lucia@risc1.lrm.fi.cnr.it

30th ANNUAL INTERNATIONAL MEETING: "ESR SPECTROSCOPY OF RADICALS IN ORGANIC AND BIOLOGICAL SYSTEMS" in conjunction with the 5TH INTERNATIONAL SYMPOSIUM ON SPIN TRAPPING: "APPLICATIONS IN CHEMISTRY, BIOLOGY AND MEDICINE", April 6-10, 1997, Lancaster, UK.

The 30th meeting of the ESR Group of the Royal Society of Chemistry, London will celebrate 29 consecutive years of International meetings on the topic of Electron Spin Resonance Spectroscopy. The meeting will be held at The Univ. of Lancaster, in conjunction with the 5th International Meeting on Spin Trapping. The Conference opens with a reception and dinner on Sunday evening and closes after lunch on Thursday. The organisers extend a cordial invitation to all persons interested in ESR spectroscopy in Chemistry and Biology to attend. Accommodation will be in individual rooms in a residence hall on the campus, where the lectures will take place.

The conference circular may be viewed on the internet at the following address:

### http://www.cf.ac.uk/uwcc/chemy/rowlandscc/conf.html

For more information, contact Dr. C.C. Rowlands (Secretary of the Committee of the ESR Group, Royal Society of Chemistry) Dept. of Chemistry, Univ. Wales, Cardiff, P.O. Box 912 Cardiff CF1 3TB, UK; e-mail: saccr@cardiff.ac.uk. *More program information can be found in Vol. 8 No. 1*.

# FIFTH MEETING of the INTERNATIONAL SOCIETY OF MAGNETIC RESONANCE IN MEDICINE (ISMRM), April 12-18, 1997, Vancouver, British Columbia, Canada.

The 1997 Scientific Meeting of the International Society for Magnetic Resonance in Medicine will combine traditional and new elements of interest to both basic scientists and clinicians to provide a program to appeal to all attendees. Programs will include:

Weekend Educational Programs: Introductory and Advanced MRI: Techniques with Clinical Applications (April 12-13); Progressive Magnetic Resonance Spectroscopy (April 12-13); The Cutting Edge in Spectroscopy (April 13).

**Plenary Lectures:** The plenary lectures will be given on Monday through Friday mornings. Of particular interest is the opening session, which will consist of the Oxford Lecture on the History of MR delivered by Robert Pound. Other plenary lectures will include:

Historical Perspectives of Biomedical NMR: from Basic Physics to Physiology and Diagnosis: Toward Better Understanding of Human Disease (R. Shulman); Celebrating 25 Years of Innovation (W. Edelstein); Clinical MR Imaging: The Ultimate Diagnostic Tool (W. Bradley).

Vascular MR: Vascular Disease—a Surgeon's Perspective (C. Zarins); Methodology of MRA (D. Parker); MRS in Diagnosis (M. Prince).

MR Imaging of Cartilage: Detection of Sports-Related Cartilage Abnormalities (M. Recht); Pitfalls, Pulse Sequences and Quantitative Techniques (C. Peterfy); Cartilage Structure and Pathobiology: Practical Applications (D. Burstein).

Ischemic Heart Disease: MRS for Understanding Ischemic Heart Disease (R. Weiss); The Clinical Role of MRI in Ischemic Heart Disease (A. de Roos); Cardiac MRI Methods—Present and Future (G. Laub).

Functional MRI: Clinical Impact, Pitfalls and Potential: Neurology: Diagnosis, Prognosis and Rehabilitation (S. Zeki); Psychiatry: A New Patient Population to Image (D. Weinberger); Surgery\Radiotherapy: A Functional Road Map (M. Raichle).

Clinical Categorical Courses: Mini-Categorical Courses from April 14-18: Head and Neck Imaging; Diffusion/Perfusion. Clinical Courses: MR Physics and Techniques for Clinicians (April 14-17); The Economics of MRI: A Worldwide Perspective (April 15); Hot Topics for Practicing Radiologists (April 16).

Meeting information can be received by contacting ISMRM at info@gateway.ismrm.org.

# 7th CHIANTI WORKSHOP on MAGNETIC RESONANCE: NUCLEAR and ELECTRON RELAXATION, May 25-31, 1997, San Miniato (Pisa), Italy.

The Chianti Workshops aim to bring together scientists involved in theoretical and experimental aspects of nuclear and electron spin relaxation to study the structure and dynamics of molecules. The Chairpersons are: I. Bertini (Univ. Florence, Conference Chairman) and Z. Luz (Weizmann Inst. Science, Program Chairman). The Organizers are L. Banci (Univ. Florence), E. Gaggelli (Univ. Siena) and C. Forte (C.N.R. Pisa).

The registration fee for the Chianti Workshop is 250,000 Italian Lira for active participants and 120,000 Italian Lira for accompanying persons. The cost of accomodations (based on sharing a twin-bed room) is 800,000 Italian Lira and includes all meals.

For more information, contact one of the following: Z. Luz, Chemical Physics Dept., Weizmann Inst. Science, Rehovot 76100, Israel, **3**: 972-8-934-2020, FAX: 972-8-934-4123, e-mail:ciluz@wis.weizmann.ac.il; L. Banci, Dept. Chemistry, Univ. Florence, Via G. Capponi 7, 50121 Florence, Italy, **3**: 39-55-2757550, FAX: 39-55-2757555, E-mail: lucia@risc1.lrm.fi.cnr.it; E. Gaggelli, Dept. Chemistry, Univ. Siena, Pian dei Mantellini 44, 53100 Siena, Italy, **3**: 39-577-298008, FAX: 39-577-280405, E-mail: gaggelli@unisi.it.

## TSUKUBA NMR 97, June 5-6, 1997, Tsukuba Science City, Ibaraki, Japan.

This is a series of annual international meetings, organized in 1994. The main topic of the 1997 meeting will be "Solvation and Flexibility in Proteins." For more information contact the Organizer, Yoji Arata, Water Research Institute, Sengen 2-1-6, Tsukuba 305, Japan; \$\approx\$: 81-298-58-6183; FAX: 81-298-58-6166; E-mail: arata@wri.co.jp.

#### FIFTH INTERNATIONAL WORKSHOP ON ELECTRON MAGNETIC RESONANCE OF DISORDERED SYSTEMS (EMARDIS) and 2nd INTERNATIONAL SEMINAR ON APPLIED EPR, June 8-17, 1997, Sophia, Bulgaria.

Extensive information about these meetings can be found in the *EPR Newsletter* (Vol. 7 No. 4).

Further Information. A first circular of both meetings is

available. The Organizers request recipients to kindly fill out and return the preliminary registration form included in it 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; **3**: 3592-713-2546 or -3917; telex: 22729 echban, e-mail: NDYEPR@BGEARN.ACAD.BG.

#### TWENTIETH INTERNATIONAL EPR SYMPOSIUM at the 39th Annual Rocky Mountain Conference, August 3-7, 1997, Denver, CO, USA.

The EPR Symposium will start Sunday evening with an open house at the University of Denver EPR labs, including refreshments provided by Bruker Instruments.

In this Symposium we will emphasize different ways of looking at unpaired electron spins and the complementary information that can be obtained by different techniques. The "normal" CW experiment is most widely used, but it is not necessarily the most powerful way to answer a particular question. There are many other methods including various multiple resonance and time-domain techniques. Since this will be the 20th year for the EPR Symposium we hope to have at least 20 techniques represented.

For further information contact: Prof. Sandra S. Eaton or Prof. Gareth R. Eaton, Dept. of Chemistry and Biochemistry, Univ. of Denver, Denver, CO, 80208-2436, USA. 3:303-871-3102;

FAX: 303-871-2254; E-mail: seaton@du.edu.

## THIRD EUROPEAN ESR MEETING, August 25-29, 1997, Leipzig, Germany.

The title of this meeting is "Modern Aspects of Structure and Dynamic Investigations of Paramagnetic Systems by EPR". A list of topics for this meeting can be found in the EPR Newsletter, Vol. 7 No. 4.

For more information, contact DP Dr. Habil. Dieter Beckert, Max-Planck-Society, Research Unit "Time Resolved Spectroscopy" at University Leipzig, Permoserstr. 15, D-04303 Leipzig, Germany; **2**: 49-341-235-2630; FAX: 49-341-235-2317; E-Mail: beckert@mpgag.uni-leipzig.de.

# 7th EUROPEAN CONFERENCE on the SPECTROSCOPY of BIOLOGICAL MOLECULES (ESCBM), September 7-12, 1997, San Lorenzo de El Escorial, Madrid, Spain.

This major International Conference will focus on the structure and dynamics of biological molecules and related systems as revealed by Raman and infrared spectroscopies and other methods, particularly NMR, CD, optical absorption and fluorescence, inelastic neutron scattering, X-ray crystallography, computer graphics and molecular mechanics and dynamics. The Conference offers the opportunity to unite spectroscopists and specialists of Biochemistry, Medicine and Biology interested in the application of spectroscopic methods for life science research. The conference is sponsored by Comité Español de Espectrascopía (SEDO) and Universidad S. Pablo - CEU.

Please direct all correspondence to the Conference Chairman: Dr. P. Carmona, ECSBM'97 Chairman, Instituto de Estructura de la Materia (CSIC), Serrano 121, 28006 Madrid, Spain;

Publication of the International EPR(ESR) Society

**3**: 34-1-5616800; FAX: 34-1-5645557;

E-mail: pcarmona@pinar1.csic.es;

Internet: http://www.uned.es/convoca/ecsbm97.htm.

SECOND INTERNATIONAL CONFERENCE on BIORADICALS and FIFTH INTERNATIONAL WORKSHOP on ESR(EPR) IMAGING AND *IN VIVO* ESR SPECTROSCOPY, October 12-16, 1997, Yamagata, Japan.

The conference will treat all aspects of bioradicals, with special attention to ESR spectroscopy. The following subjects comprise the main scientific scope:

- A. Bioscience of reactive oxygen species including Chemistry, biochemistry and pathophysiology of bioradicals; Redox regulation and signal transduction; Antioxidants and food science.
- B. Biological applications of ESR spectroscopy, e.g., ESR imaging; *In vivo* applications of ESR; Biological applications of ESR methodologies.
- C. Other topics to be determined

To receive a circular, contact Dr. Hiroaki Ohya-Nishiguchi, Institute for Life Support Technology, Yamagata Technopolis Foundation, 2-2-1 Matsuie, Yamagata 990, Japan;

**2**: 81-236-47-3134; FAX: 81-236-47-3149;

E-mail: ohya@ymgt-techno.or.jp.

## FIFTH INTERNATIONAL CONFERENCE ON SPIN CHEMISTRY, October 26-31, 1997, Jerusalem, Israel.

An official circular will be available shortly. For more information please contact Haim Levanon, Dept. Physical Chemistry, The Hebrew University, Jerusalem, 91904 ISRAEL. **2**: 972-2-658-5544; FAX: 972-2-618-033;

e-mail: levanon@vms.huji.ac.il.

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

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

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

For further information on the XVIIIth ICMRBS, please contact Prof. M. Kainosho, Dept. Chemistry, Tokyo Metropolitan Univ. (TMU), Hachioji, Tokyo, Japan;

**3**: 81-426-77-2544; FAX: 81-426-77-2525;

e-mail: kainosho@raphael.chem.metro-u.ac.jp.

## ADDITIONAL CONFERENCE UPDATES ON WORLDWIDE WEB.

The EPR Newsletter web page contains the latest information on conferences for which notices arrived after the publication deadline. The web address is:

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

# POSITIONS AVAILABLE & WANTED

### **POSITIONS AVAILABLE**

Post-doctoral position available at the University of Pennsylvania, Department of Biochemistry, Philadelphia, PA, USA. One post doctoral position is now available in my laboratory to those who are interested in the structure/function studies on electron-transfer and energy-coupling mechanisms. Our research projects include bacterial and mitochondrial transmembrane complexes focusing on the NADH-quinone, succinate-quinone, and quinol-cyt.c oxidoreductase systems. Electron paramagnetic resonance spectroscopy is used as a major research technique in my laboratory, in combination with other methods such as spectrophotometry or potentiometry. We also conduct collaborative projects with other laboratories with expertise in molecular biology and other spectroscopic techniques such as electron nuclear double resonance (ENDOR). [Sample reference: Eur. J. Biochem., 230, 538 (1995): J. Biol. Chem., 270,18264 (1995): FEBS Letts, 370, 83 (1995): Biochemistry, 35, 7834 (1996).] Applicants for this position should have experience with standard EPR techniques. Interested individuals should send curriculum vitae and addresses of three references to Prof. Tomoko Ohnishi, Johnson Research Found., Dept. Biochemistry and Biophysics, Medical School, Univ. Pennsylvania, 37 Hamilton Walk, Philadelphia, PA 19104-6089. Fax: 215-573-3748: E-mail: ohnishi@mail.med.upenn.edu. The University of Pennsylvania is an Affirmative Action/Equal Opportunity Employer.

Postdoctorial fellowship available, NIEHS/NIH, Research Triangle Park, NC, USA. Biological ESR spectroscopist for investigations into protein-derived radicals, *in vivo* detection of radicals, and/or nitric oxide complexes. Less than five years postdoctorial experience with a Ph.D. in chemistry, biochemistry, pharmacology, or toxicology. Please send curriculum vitae to Ronald P. Mason, Free Radical Metabolite Workgroup Leader, NIEHS/NIH, P.O. Box 12233, Research Triangle Park, NC, 27709, USA; **2**: 1-919-541-3910; FAX: 1-919-541-5737.

Postdoctoral position in Electron Spin Resonance available, University of Florida, Gainesville, FL, USA. The University of Florida in Gainesville/Florida invites applications for a postdoctoral research associate position with an early 1997 starting date. The successful candidate will help to set up, maintain, and operate a multi-user ESR/ENDOR/ODMR spectrometer (new Bruker FT-ESR/ENDOR). His/her research focus will be on the development of new ODMR and ODENDOR methodology and its application in the areas of biophysics and/or materials science. He/she will also participate in the training of users from various research groups on campus and help them in the use of the instrument and interpretation of spectra.

Candidates must possess a Ph.D. in physics, chemistry, or related disciplines and have a strong background in pulse ESR (FT and/or ESEEM), or pulse ENDOR. He/she must be able to program in C and be familiar with an UNIX environment. Experience with Bruker equipment is a plus but not essential.

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

Excellent written and verbal communication skills are necessary, as is interest in working in a multi-disciplinary research laboratory.

We have a major research collaboration with the National High Magnetic Field Laboratory in Tallahassee/Florida which gives the candidate the opportunity to perform complementary ESR studies at fields up to 25 Tesla and frequencies up to 3 THz.

The position is available for 2 years, initially. Salary will range between US\$ 25,000 and 30,500, depending on experience. For further information, contact Prof. Angerhofer, : 1-352-392-9489, FAX: 1-352-392-0872; E-mail: alex@chem.ufl.edu. Send CV, and arrange for 2 letters of support to be sent to: Dept. Chemistry, c/o A. Angerhofer, Univ. Florida, Box 117200, Gainesville/FL 32611-7200, USA.

Ph.D. Studentship Available, University of Essex, UK. I currently have a BBSRC PhD studentship available for a UK student with a II(i) or better degree (or who expects to get one). A II(ii) + Msc. would also be possible. The studentship would be in biomedical EPR spectroscopy, probably relating to some aspect of nitric oxide interaction with biological systems, although the detailed project could be the subject of negotiation. Anyone interested or who knows someone who might be interested should e-mail me or look for further details on my Web page. Contact Dr. Chris Cooper, Dept. Biological and Chemical Sciences, Central Campus, Univ. Essex, Wivenhoe Park, Colchester CO4 3SQ, UK; ☎: 44-1206-872752; FAX: 44-1206-872592; E-mail: ccooper@essex.ac.uk; Web page is:

http://www.essex.ac.uk/bcs/staff/ccooper/cooper.html

Position Available in Interactive Computer Simulation/Visualisation of ESEEM and Pulsed ENDOR Spectra, University of Queensland, Australia. The Centre for Magnetic Resonance and the Department of Mathematics are collaborating with the EPR Division of Bruker Analytische Messtechnik in the development of an interactive computer simulation/visualisation software environment for the analysis of randomly oriented ESEEM and pulsed ENDOR spectra. Facilities at the University of Queensland include a multifrequency (Q-, X- and S-band) EPR spectrometer, and extensive computational facilities. Bruker will provide expertise in relation to their Xepr data acquisition/manipulation software environment and access to pulsed EPR and ENDOR facilities.

We are seeking an experienced and highly motivated scientist with a PhD in physics, chemistry or a closely related discipline with two or more years' experience in the areas of pulsed EPR spectroscopy to join our multidisplinary research group in the University of Queensland. The successful candidate will have an in-depth understanding of the theoretical aspects of pulsed EPR or NMR spectroscopy and be able to competently programme in C. Strong written and verbal communication skills are essential for the formal documentation of research results and productive interactions in a multi-disciplinary research team environment. The position is available for three years beginning in early 1997. The successful applicants' salary will be commensurate with the applicants' background within the range \$30,537-\$38,587 (Australian). Superannuation benefits and a one way airfare to Brisbane will also be provided. There will be opportunities for attending international conferences and visiting Bruker.

Applicants should immediately forward a resume, including the names and addresses of three professional referees to: Dr. Graeme Hanson, Centre for Magnetic Resonance, The University of Queensland, St. Lucia, Queensland, Australia, 4072. **2**: +61-7-3365-3242, Fax: +61-7-3365-383, E-mail: Graeme.Hanson@CMR.uq.edu.au.

Research Associates/Post-doctoral Positions at the EPR Center for the Study of Viable Biological Systems, Dartmouth Medical School, Hanover, NH, USA. The EPR laboratory at Dartmouth has several immediately available openings for research and development in the EPR Center and/or in the program project for the development and application of oxygen-sensitive paramagnetic materials. opportunities/needs range from instrumental development of low frequency EPR spectroscopy to biological applications in animals to studies in isolated cell systems. There are specific needs for individuals with strong backgrounds in engineering/instrument development and for an individual with excellent skills in cell culture. The initial appointments will be made for 1 year with the possibility of extensions up to 5 years or longer. Candidates should submit a complete CV including a description of prior experience and areas of research interests, and should arrange for 3 letters of reference to be sent directly to Prof. Hal Swartz, Dartmouth Medical School, 7785 Remsen, 03755 USA; E-mail: NH. Hanover, harold.swartz@dartmouth.edu; FAX: 1-603-650-1130.

Research Assistant in Electron Paramagnetic Resonance, National University of Singapore. The Department of Chemical Engineering at the National University of Singapore invites applications for a research assistant position. The successful candidate will be involved in a research program of investigating electron transport through liquid membranes with redox active properties. Fluent English and knowledge of EPR is a plus. Preference will be given to a candidate holding a Ph.D. (or equivalent) in physical chemistry/biochemistry or related fields, although persons with M.S. degree are also welcome to apply. Initial appointment will be made for a half or one year with a potential renewal. Level of compensation will be in accordance with qualification of the candidate. Candidates should submit a curriculum vita and arrange for three letters of reference to be send to: Dr. Nikolai Kocherginsky, Department of Chemical Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore, 119260. 2: 65-7715083; FAX: 65-7791936; E-mail: Chenk@leonis.nus.sg.

Visiting Woman Professor, Linkoping University, Linkoping, Sweden. We can offer a temporary visiting professorship for a woman scientist with a background in EPR. The position is for 12 months. Costs, up to 0.85 MSEK or \$125,000 will be covered by a grant from the Swedish National Science Research Council. The grant can be used for salary and travel. At present the research is focused on structural and dynamical investigations of radical ions, in matrices and on surfaces, of the structure of paramagnetic species in Cu-exchanged zeolites, and structural and dynamic studies of protein folding using spin labels. In addition some single studies of radiation damage are performed as well as studies of EPR dosimetry. The research can be in any of these or other fields

Publication of the International EPR(ESR) Society

proposed by the candidate, subject to limitations set by available equipment. We have at present a CW Bruker 200 EPR and ENDOR spectrometer and will have a Bruker 380 pulsed EPR and ENDOR spectrometer installed at the end of 1996. Please contact Anders Lund for information: Dept. Physics and Measurement Technology, Linkoping Univ., S-581 83 Linkoping, Sweden; ع: 46-13-282665; FAX: 46-13-132285; E-mail: ald@ifm.liu.se; World Wide Web:

http://www.ifm.liu.se/Chemphys.

## **POSITIONS WANTED**

Transition Metal Ion Spectroscopist [Optical, IR, EPR] spectroscopist seeks Postdoctoral Position/Academic Positions. Research Experience: EPR and optical studies of Transition Metal Bearing crystals studied extensively. Have the experience to record the EPR spectra experimentally. Currently working to develop the simulation programs for knowing the microwave frequency range to detect the EPR signals. Well acquinted in preparation of high Tc Superconducting Ceramics and other crystals by different techniques and their characterization by optical and electrical measurements. Publications: Journal publications: 13 (Thirteen); Conference papers: 8 (National), 3 (International). Qualifications: M.Sc., M.Phil., Ph.D., M.Sc. Specialisation: Solid State & Vacuum and thin film physics, M.Phil: Characterization of Ceramic Raw Materials by Spectroscopic and Electrical Measurements, 1990 from S.V.University, Tirupati, INDIA. Ph.D.: Electrical and Spectroscopic Studies on Transition Metal Bearing Crystals and Oxide Ceramics, 1994 from S.V.University, Tirupati, India. An early reply in this regard is highly solicited.

Contact: Dr. Madhu Sudhana Budamagunta, RA, Dept. of Physics and Materials Science, City Univ. Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong; **3**: 852-2788-7707 (Office), 852-2686-9981 (Residence); FAX: 852-2788-7830;

E-mail: apmadhu@cityu.edu.hk.

# EQUIPMENT & SUPPLIES EXCHANGE

#### WANTED: BENCH-TOP EPR SPECTROMETER

We are looking for a bench-top EPR spectrometer, like an E-3. Does anyone have or know of an EPR which is collecting dust? We are short on cash, so price is important. Please contact Prof. Lew Cary, Dept. Chemistry, Univ. Nevada, Reno, NV 89506 USA; \$\mathbb{z}: 1-702-784-6019; E-mail: lcary@chem.unr.edu.

#### 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; \$\alpha/FAX: 1-773-728-6570.

#### 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;

**3**: 1-864-294-3372; FAX: 1-864-294-3559; E-mail: knight lon/furman@furman.edu.

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

JEOL TE2000 SPECTROMETER

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 KHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a conversion kit to convert Varian field control units to voltage-controlled scan operation. A 6 digit 1 ppm frequency counter is available in X-, C-, S- or L-band or Megahertz versions. Complete microwave/RF bridges from 150 MHz to L-, S-, or C-band are available from designs previously built and tested at the Univ. Denver. Contact: Richard W. Quine,  $\Rightarrow$ : 1-303-871-2419 or e-mail: rquine@du.edu.

#### FOR SALE: VARIAN SYSTEM

Resonance Instruments presently has available:

- 1) a E110 Q-band Bridge with cavity
- 2) replacement Klystrons for Varian EPR Bridges (at reduced prices)
- Model V4533 VARIAN EPR TE011 mode, rotating cylindrical cavity
- 4) VARIAN general purpose cavity E231
- 5) VARIAN V4500-41A low/high power microwave bridge with new klystron—excellent condition
- 6) X-band DEWAR probe outfitted with a tuner and with stainless steel waveguide

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

#### **AVAILABLE: TWO IBM 9000 COMPUTERS**

We have two IBM 9000 computers that were used to control our IBM (Bruker) EPR spectrometer, including the double floppy disk drive and a hard disk, to give away. They were still working well when we switched them off about two years ago. For information, contact: Eicke Weber, Materials Science Division, Berkeley Lab, and Dept. Materials Science and Mineral Engineering, Univ. California, 587 Evans Hall, Berkeley, CA 94720, USA; 2: 1-510-642-0205;

FAX: 510-642-2069; E-mail: weber@garnet.berkeley.edu; www: http://www.mse.berkeley.edu/faculty/weber/weber.html

#### AVAILABLE: VARIAN MAGNET AND POWER SUPPLY

V-3800 magnet, 15" diameter pole pieces. Could be adapted to sweep up to 2.4 T (24,000 G) or more. Narrow gap, originally used in XL-100 NMR spectrometer. Free to anyone who will pay cost of removal and give it a good home. Contact Mark Nilges at the IERC, 190 MSB, MC-714, 506 S. Mathews Ave., Urbana, IL 61801, USA. ع: 1-217-333-3969; FAX: 1-217-333-8868; E-mail: nilges@uiuc.edu

## WANTED: USED X-BAND MICROWAVE BRIDGE

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

## **ANNOUNCEMENTS**

#### MAILING LISTS FOR SCIENTIFIC MEETINGS

If you are planning a scientific conference, you may contact an officer of the IES or the IERC (address at left) to obtain a list of the 1,400+ Society members for use in issuing invitations. If you would like mailing labels, Martha Moore, who provides secretarial support for the Society, can do this at cost -- approximately \$50.00 per 1,000 (includes cost of labels, postage and, if you wish, a disk copy of the list in ASCII format). Labels for the entire database (over 3,800 members and non-members) would cost about \$200.00.

#### MEMBERSHIP INFORMATION AVAILABLE ON THE WEB

This year, a list of all members whom the IES records show as having paid dues in 1994, 1995, and/or 1996 was put 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 update the list monthly; please allow time for recent payments to be placed on the list. 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 dues payment form is on this web site along with methods to pay dues, depending on where in the world you are located.

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

#### AREA CODES CHANGING IN CHICAGO

Some members with the area code 312 (for Chicago, Illinois, USA) will now have a new area code, 773. This change will affect about half of the phone and fax numbers in the old 312 code area so feel free to contact us at the IERC if you wish to verify numbers.

#### ABOUT THIS PUBLICATION

- •This publication is the official newsletter of the International EPR(ESR) Society. It is supported by the Society, by corporate and other donors, and by the Biomedical Technology program of the Division of Research Resources in the U.S. National Institutes of Health through the Illinois EPR Research Center at Urbana.
- ·Editor: R. Linn Belford
- ·Assistant Editor, Becky Gallivan
- •Typography: Martha Moore.
- •The EPR Newsletter is produced with the cooperation of these 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 address: cfelix@post.its.mcw.edu WWW: http://www.biophysics.mcw.edu/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 address: peisach@aecom.yu.edu WWW: http://spin.aecom.yu.edu

#### EPR Center for the Study of Viable Biological Systems,

Prof. Hal Swartz, Director

Prof. Ted Walczak, Associate Director Dartmouth Medical School, Dept. of Radiology 7785 Remsen, Hanover, New Hampshire 03755-3863, USA.

**=**: 603-650-1784. FAX: 603-650-1130.

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

#### Illinois EPR Research Center (IERC),

Prof. R. Linn Belford, Director; Prof. Robert B. Clarkson, CoDirector; Prof. Peter G. Debrunner, Assoc. Director, Prof. Mark J. Nilges, Asst. Director, Prof. Alex I. Smirnov, Laboratory Manager; Ms. Becky Gallivan, Asst. to the Directors; Ms. Martha Moore, Secretary.

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

**☎**: 217-244-1186. FAX: 217-333-8868.

E-mail address: ierc@uiuc.edu or rlbelford@uiuc.edu WWW: http://ierc.scs.uiuc.edu

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

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

Publication of the International EPR(ESR) Society

## The International EPR(ESR) Society Would Like to Thank the Following Corporate Sponsors for their Continued Support:

American Inst. Physics

Bruker Instruments, Inc.

Cambridge Isotope Laboratories

**CPI** 

Cryo Industries America, Inc.

**GMW** Associates

JEOL USA, Inc.

Medical Advances, Inc.

Norell, Inc.

Oxford Instruments

Oxis International

Research Specialties

Resonance Instruments Inc.

Resonance Technologies, Inc.

Scientific Software Services

Sumitomo Special Metals

Summit Technology Inc.

Wilmad Glass Company, Inc.

Volume 8, Number 4

Page 1

Spring, 1997



JAN SCHMIDT
PHOTO COURTESY OF
RALPH WEBER

# Profile of Jan Schmidt, IES Silver Medalist—

Schmidt's scientific achievements, which earned him the Society's Silver Medal for Physics and Instrumentation in 1995, appear to reflect the advantages of a varied career in his early days. After obtaining a master's degree in experimental (i.e. solid state) physics at the University of Amsterdam, Schmidt's formal university studies were interrupted for six years. First he fulfilled his

military service requirements by working for two years in the research laboratory of the Dutch defense organization, where he had the opportunity to familiarize himself with modern microwave techniques. Subsequently, he joined the Koninklijke/Shell laboratorium, Amsterdam, which posted their new employee for a training period of two years in the physics laboratory of the prestigious Ecole Polytechnique in Paris. Here Abragam's "long-legged spinner," Ionel Solomon, guided him into the secrets of EPR, and together they investigated phosphorus centers in silicon. Besides, Schmidt got a thorough education in the French way of life, and Jan loves to recount how he participated in a protest march of striking scientists, clad in laboratory coats, on the streets of Paris.

Back at Shell, Schmidt worked for a couple of years on the investigation of transition metal ions such as Ti<sup>3+</sup> in catalysts by means of EPR and ENDOR. But when the interdisciplinary Centre for the Study of the Excited States of Molecules at the University of Leiden is founded in

- Editor: R. Linn Belford, Urbana, lL
- •Assistant Editor, Becky Gallivan, Urbana, IL
- Typography: Martha Moore, Urbana, IL.
- This, the official newsletter of the International EPR(ESR) Society, is supported by the Society, by corporate and other donors, and by the ational Center for Research Resources in the U.S. National Institutes of Health. For additional information including how to contact the editor, see the box "About This Publication" on p. 29.

#### FELLOWS OF THE INTERNATIONAL EPR(ESR) SOCIETY

- ANATOLE ABRAGAM
- BREBIS BLEANEY
- CLYDE HUTCHISON
- ALEKSANDR PROKHOROV
- GEORGE FEHER
- Ralph Hahn
- . J. H. VAN DER WAALS
- OR PROKHOROV SAMUEL WEISSMAN

# 1997 IES AWARD WINNERS NAMED

Harden M. McConnell—
GOLD MEDAL

Anatole Vanin—

SILVER MEDAL FOR BIOLOGY/MEDICINE

Hanns Fischer—

SILVER MEDAL FOR CHEMISTRY

Roger Isaacson—

SILVER MEDAL FOR PHYSICS/INSTRUMENTATION

Robert Bittl—

YOUNG INVESTIGATOR AWARD

1967, Schmidt opts for an academic career -- to begin on the track towards a Ph.D. degree. The initial program of the Center was focused on the challenge to detect electron spin transitions of photo-excited triplet states of organic molecules by optical methods in zero field, and to investigate coherence phenomena in these states. The first two theses coming from the Center bear witness to the realization of these goals and of the great competence of their authors: Jan Schmidt's *Modulation of* 

#### IN THIS ISSUE

Profile of Jan Schmidt, IES Silver Medalist in Physics & Instrumentation 1-2
1997 IES Awards Announcement 1
Profile of Gunnar Jeschke, 1996 IES Young Investigator 2-3
VOCVOGSKV Prize Announced
International EPR(ESR) Society Affairs
From the Editor (R.L. Belford), From the President (J.R. Norris),
Nominations Open for IES Secretary, Asia-Pacific EPR/ESR
Society, Credit Card Payments, IES Awards
The Computer Corner (K. Madden, R. Morse, et al.)
EPR Specialist Vignettes (A. Schweiger, ed.) 8-10
EPR Monitoring of Plants & Lichens (Jezierski & Bylinska)
Building the Perfect Beast (C. Bender)
Tips & Techniques 13.15
Replacing Varian Spectrometer Recorder Cables (Belford & Wentz)
An Improved Simple Device for the Precise Positioning of a Sample at
Arbitrary Points of the Intracavity Space (Maúr & Morris)
Conference Report First Asia-Pacific EPR/ESR Symposium 15-19
Books & Proceedings
Notices of Meetings 20-26
Positions Available & Wanted 26-27
Equipment & Supplies Exchange 27-28
Announcements (Mailing lists; Info. on WWW; E-mail updates) 28-29
Special Offer for IES Members - "Applied Magnetic Resonance"
About this Publication ( <i>The Masthead</i> )

Phosphorescence by Microwaves and Wiebren Veeman's (now an expert on solid-state NMR and professor at the University of Duisberg, Germany) Level Anticrossing and Cross-Relaxation in Phosphorescent Organic Crystals.

After obtaining his Ph.D. degree in 1971, Jan is intrigued by the use of pulsed experiments to probe the dynamics of the optical pumping cycle of polyatomic molecules and he succeeds in observing electron-spinecho signals from a short lived photo-excited triplet state. Subsequently, as a postdoc with R.G. Brewer at the IBM Research Laboratory at San Jose, he carries out infra-red photon-echo experiments on ro-vibronic transitions of small molecules in the gas phase.

In 1974 Schmidt was appointed professor at the University of Leiden. Whereas, initially, Jan Schmidt in his work reaped the benefits of the new tools he and his colleagues had developed for the study of the photophysics of organic molecules, his interests later widen to include inorganic systems, such as defects in semiconductors and paramagnetic centers in AgCl - the intriguing material at the basis of photography. And, in a collaboration with W.E. Moerner (IBM) he recently succeeded in observing spin transitions in the triplet state of single molecules.

Most rewarding proves the high-frequency pulsed EPR project initiated by Jan Schmidt in the late eighties. With the help of a very able technician, J.A.J.M. Disselhorst, a 95 GHz pulsed EPR/ENDOR spectrometer has been built which proves a "winner". The instrument, because of the high microwave frequency and strong magnetic field, has two very attractive features: (1) a high sensitivity (10<sup>7</sup> spins per gauss) which allows one to study minute samples; (2) a high resolving power in the case of amorphous samples with an anisotropic g tensor. Two recent Ph.D. theses from Jan's group provide nice illustrations of what can be achieved: J.W.A. Coremans, W-band Electron Spin Echo Spectroscopy of Azurin and M.T. Bennebroek, High-field Electron Nuclear Double Resonance Spectroscopy on Photo-induced Centers in Silver Halides. For a reader of these theses (or the corresponding papers) it is no wonder that many clients of Bruker A.G. have decided to follow Jan's lead!

J.H. van der Waals Leiden University



GUNNAR JESCHKE PHOTO COURTESY OF ARTHUR SCHWEIGER

## Gunnar Jeschke: IES Young Investigator Award for 1996—

The Young Investigator Award 1996 of the IES has been presented to Dr. Gunnar Jeschke in recognition of his significant contributions to EPR spectroscopy, and in particular to the development of novel one- and two-dimensional pulse EPR experiments. Gunnar Jeschke was born in 1966 in Cottbus,

Germany. Already during high school (Oberschule), he was honored with the 2nd prize in the XIV International Chemistry Olympiad in Romania. From 1988-1992, he studied chemistry at Dresden Technical University; he graduated with a diploma thesis in the field of solid-state NMR and was awarded the Lohmann Medal. Gunnar then spent one year at the Institute of Physical and Chemical Research (RIKEN), Japan, where he studied magnetic field effects on chemical reactions by laser flash photolysis and time-resolved EPR. In November 1993 he joined my research group in the Physical Chemistry Laboratory at ETH, Zürich, as a graduate student. He finished his doctoral thesis with the title: "New Concepts in Solid-State Pulse Electron Spin Resonance" in the Spring of 1996. During his time as a graduate student Gunnar Jeschke designed an impressing number of very promising new one- and two-dimensional pulse EPR and ENDOR techniques with the objective to simplify or disentangle the spectra and to improve the sensitivity of known pulse EPR schemes. Among other methods he developed are these:

## **GMW** Associates

- Laboratory Electromagnets & Power Supplies
- Precision Hall Effect Teslameters
- Digital NMR Teslameters
- Digital Voltage Integrators
- Precision Current Transducers

Specializing in Magnetic Measurements and Electromagnet Systems PO Box 2578, Redwood City, CA 94064 USA. Tel (415)802-8292 Fax (415) 802-8298

Publication of the International EPR(ESR) Society

#### **Attention: Oxidative Stress Researchers**

## **New Spin Trap - DEPMPO** For differentiating O2 and OH radicals

• 15 times more stable than DMPO superoxide adduct Unambiguous fingerprint of scavenged free radical Samples can remain frozen without damage or loss of ESR signal

#### Call for Free Catalog:

Assavs Fine Chemicals Proteins

Antibodies

Innovative technologies for oxidative stress research™



voice: USA 1-800-547-3686 voice: France 33 1 49 80 4565 home page: http://www.oxis.com email: info@oxis.com

- ESEEM with matched pulses, a technique for enhancing the modulation depth.
- Hyperfine decoupling in ESEEM and ENDOR spectroscopy, which allows one to correlate hyperfine-coupled and hyperfine-decoupled nuclear frequencies.
- Zero-field ESEEM and pulse ENDOR methods to display highly resolved spectral features even for disordered systems.
- Hyperfine spectroscopy for the direct measurement of hyperfine frequencies and their correlation to the nuclear frequencies.
- Chirp ENDOR spectroscopy in one and two dimensions, a pulse ENDOR approach with increased sensitivity and resolution.
- Nutation-frequency correlated EPR spectroscopy to disentangle complicated field swept EPR spectra into a nutation-frequency dimension.

After this short but very fruitful period of time in the world of the electron spins Gunnar Jeschke will now devote his attention to methodology and applications of solid state NMR. Prof. Arthur Schweiger

Lab. Physikalische Chemie, ETH-Zentrum, Zürich

## Voevodsky Prize Announced—

This year the international science community is celebrating Academican Voevodsky's 80th anniversary. Academician Vladislav Vladislavovitch Voevodsky (1917-1967) is one of the most outstanding and brilliant representatives of the school of scientists who created chemical kinetics and chemical physics as a science of physics and chemistry of elementary chemical reactions. He has made a very important contribution to the study of mechanisms of gaseous branching chain reactions, to the investigation of reactions of hydrocarbon cracking, to the investigation of heterogeneous reactions of radicals and atoms.

In memory of Academician V.V.Voevodsky and in connection with his 80th anniversary, the Institute of

Chemical Kinetics and Combustion of the Siberian Branch of Russian Academy of Sciences, the International Tomographic Center, and the Center of Chemical Radiospectroscopy of Active Intermediates (Novosibirsk) establish the Voevodsky Prize.

The Voevodsky Prize is recognized by the Ampère Society, International EPR(ESR) Society, Committee of the European Federation of ESR groups, ISMAR, and Novosibirsk State University.

The first Voevodsky Prize (2000 USD in 1997) and diploma will be awarded to a Russian scientist in 1997 during the conference "Physics and Chemistry of Elementary Chemical Reactions" dedicated to the memory of V.V. Voevodsky. This conference will be held in Chernogolovka, Moscow region. September 29 -October 3, 1997. (See "Notices of Meetings" in this issue for details.)

Starting in 1997, the Voevodsky Prize is awarded once in two years either at the session of the Scientific Council of Institute of Chemical Kinetics and Combustion or during the conference dedicated to memory of V.V. Voevodsky. An Awardee must participate in these meetings and deliver a lecture on his scientific work.

Awarding of the Voevodsky prize is based on a competition. Candidates are nominated by scientific institutes or by scientists in different research fields related to radiospectroscopy studies of mechanisms of chemical reactions and the structure of active intermediates. The results of the competition are summed up by an Award Committee (seven members including a secretary) consisting of representatives of founders and of foreign scientists. Members of the Committee are selected by Scientific Council of the Institute of Chemical Kinetics and Combustion and are renewed each five years.

Award Committee

These are the members of the Award Committee selected for the first 5 years: 1. Yu.D.Tsvetkov (Novosibirsk) - Chairman; 2. Yu.N.Molin (Novosibirsk); R.Z.Sagdeev (Novosibirsk); 4. V.I.Goldansky (Moscow); 5. J.R.Norris (Chicago); 6. K.A.McLauchlan (Oxford); 7. I.V. Chalova (Novosibirsk) - Secretary. The members of the Award Committee can not participate in the competition.

The Award Committee would welcome submitted nominations, which they hope to receive by August of 1997. Each nomination should be accompanied by a brief summary of the achievements of the nominee, covering no more than two pages.

Nominations should be mailed to Dr. I.V. Chalova, Secretary of the Award Committe, Institute of Chemical Kinetics and Combustion RAS, Novosibirsk-90, Russia 630090, or by E-mail: <Tsvetkov@ns.kinetics.nsc.ru> or <tsvetkov@ kinetics.nsk.su>.

## **♦ IES AFFAIRS ♦**

ANNOUNCEMENTS AND
REPORTS FROM THE INTERNATIONAL
EPR SOCIETY

### From the Editor—

This is the once-a-year public edition of the EPR Newsletter. If you are a member of the International EPR (ESR) Society, you're used to receiving at least four issues per year. If you are not a member, we hope you'll join. Membership gives you a lot, including an annual Directory issue of the Newsletter with updated contact and research interests listings for your colleagues worldwide. It doesn't cost much, and there are regional treasurers around the world to accept the modest dues in local currencies. You'll find forms for joining the Society at the end of this issue as well as on our Web site: http://ierc.scs.uiuc.edu/IES.html. I want to mention another benefit available only to IES members - the right to subscribe to the excellent journal APPLIED MAGNETIC RESONANCE, edited by our distinguished colleague Prof. Kev Salikhov, for only about 10% of its regular price! You will find further information about this offer on page 29 of this issue.

In the two previous editions of the newsletter, there were pictures of IES Awardees. I am delighted to thank Prof. Arthur Schweiger for taking and furnishing these photographs.

R. Linn Belford, Editor

### From the President—

The International EPR(ESR) Society has enjoyed a remarkable birth and initial growth. The Society as guided by Presidents Swartz, McLauchlan and fellow officers has served as a vehicle to promote EPR(ESR) and to encourage worldwide recognition of EPR(ESR). Several valuable services are provided by the Society,

## WILMAD GLASS Co.

is a CONTRIBUTOR to the International EPR Society

"Serving the Spectroscopic Aftermarket"

EPR Glassware/Quartzware. Sample cells. Dewars.

Address: Route 40 & Oak Rd.

Phone/FAX:

Buena, NJ 08310, USA 609-697-3000 / 609-697-0536

including this highly successful and useful EPR Newsletter. In addition, a variety of awards are sponsored by the Society. Previously these awards have been presented at the EPR symposium of the Rocky Mountain Conference. Gareth and Sandy Eaton have performed a wonderful service to the EPR community by providing a platform to honor our awardees. Their hosting this annual EPR meeting is truly remarkable and deserves exceptional recognition. We are most grateful for their tireless work on behalf of the EPR(ESR) community and especially on behalf of the Society.

We are now entering a critical phase of the International EPR(ESR) Society with two main concerns. First, we must continue to grow by expanding our membership worldwide. Only this growth will result in a true global society. Already we have members in 55 countries. To acknowledge the global nature of the International EPR(ESR) Society this year's awards will be presented in Europe at the III. European ESR Meeting, August 24-29, 1997 in Leipzig, Germany. We are most fortunate and appreciative that Dr. Dieter Beckert, Dr. Marina Brustolon and organizers of this III. European ESR Meeting have agreed to host the award presentations. Furthermore, I hope that the International EPR(ESR) Society can develop a policy where the awards will be presented at different meetings around the world, further contributing to the internationalization of the Society. Other steps intended to spread the operational procedures of the Society are planned to further "globalize" the Society. It is my intention that the active participation of the International EPR(ESR) Society will promote the field of EPR(ESR) in a healthy and competitive manner.

That EPR(ESR) is thriving worldwide is evidenced by the Voevodsky Prize recently sanctioned by the Scientific Council of the Institute of Chemical Kinetics and Combustion, Siberian Branch, Russian Academy of Science. In memory of Professor Vladislav V. Voevodsky, this prize is for outstanding contributions to the "mechanisms of chemical reactions, structure and properties of active intermediates, elementary acts in photo- and radiation chemistry." For more information on the Voevodsky Prize and its associated meeting "Physics and Chemistry of Elementary Chemical Processes" September 29th-October 3d, 1997 in Chernogolovka, Russia, see additional details in this newsletter.

Second, we must maintain our present status via our dues-paying membership. Without these dues the International EPR(ESR) Society will have too few resources to represent properly its membership base. These fees are used to support this newsletter, to support the awards and to maintain the database that currently

Publication of the International EPR(ESR) Society

includes the names and addresses of more than 1400 members. Of those listed in the database, only 549 are current with their dues. So please help maintain the International EPR(ESR) Society and its continued success by paying the small annual fee. Dues can now be paid by credit card (Visa and Mastercard); details can be found in this issue of the Newsletter. To check whether you are up to date in your payment of dues you can log in on the World Wide Web site of the International EPR(ESR) Society, http://ierc.scs.uiuc.edu/IES.html.

The time has also come to choose a new Secretary for the International EPR(ESR) Society. The current Secretary, Arthur Schweiger, is scheduled to step down soon. The secretary's job involves a considerable amount of time and work. Arthur has done an amazing job and will be most difficult to replace. I would like to thank him for all that he has done for the International EPR(ESR) Society and especially for all the help he has given to me. In keeping with the globalization of the IES, Keith McLauchlan and committee have chosen Australian John Pilbrow as the next Secretary. John is well known to the EPR community and is an excellent choice for this important and difficult position. I welcome John's assistance and advice and look forward to working with him. Also, council ballots are overdue, so please mail in your ballot from Newsletter Vol. 8 #3.

Information about the EPR Newsletter may be obtained at the Newsletter's World Wide Web site http://ierc.scs.uiuc.edu/news.html. Contributions to the EPR Newsletter are also welcome and should be sent to Ms. Becky Gallivan at College of Medicine, 190 Medical Sci. Bldg., Urbana, IL 61801 USA; E-mail: ierc@uiuc.edu.

Finally, I would like to invite everyone to participate fully in the International EPR(ESR) Society. Any suggestions can be sent to me at j-norris@uchicago.edu.

Sincerely, Jim Norris

## Pilbrow New IES Secretary—

We are pleased to announce the appointment of John R. Pilbrow of Monash University, Clayton, Victoria, Australia as Secretary of the Society for three years commencing on September 1st, in succession to Arthur Schweiger. We are grateful to Arthur for having filled the post for four years so as to introduce a stagger into the appointments of some of the Senior Officers, and even more grateful for the excellent job he has done.

John Pilbrow has served the Society nobly already as Regional Treasurer in Australia, and his appointment is an example of the Society's wish to distribute its official positions widely geographically. We are very much aware

## 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

of our members in countries which have not yet been given such representation, and expect to bring forward proposals for an enlarged Main Committee to address this.

As immediate Past President (to whom the task falls to ensure that new officers are found) Keith McLauchlan apologises that on this occasion it has not been possible to hold a ballot of members, John's name having emerged by consultation.

# Asia-Pacific EPR/ESR Society Organized—

During the First Asia-Pacific EPR/ESR Symposium, held January 20-24, 1997 in Hong Kong, the Inaugural Meeting of the Asia-Pacific EPR/ESR Society was held with 62 researchers attending. A welcome address from Prof. Jim Norris, President of the International EPR/ESR Society, was read at the meeting and the following persons were selected as the Provisional Council:

### PROVISIONAL OFFICERS:

President: Prof. Czeslaw Rudowicz (Hong Kong)
Vice-President: Prof. Asako Kawamori (Japan)
Secretary: Dr Y.Y. Yeung (Hong Kong)
[nominated later by the President]

Treasurer: Prof. Hiroaki Ohya-Nishiguchi (Japan)

## PROVISIONAL REPRESENTATIVES (AND THEIR AREAS):

Australia/New Zealand:

Japan:
Prof. Asako Kawamori
P.R.China:
Prof. R.Y. Zhan
India:
Prof. S.V. Bhat
Rep. of Korea:
Prof. S.H. Choh
Vietnam:
Prof. N.T. Nguyen
Russia (Far East):
Prof. A. Ziatdinov

During this meeting, plans were made for an official election to be held, for the provisional officers to draft a constitution and for a database of potential members from the Asia-Pacific area to be maintained.

For further information, please contact Prof. Czeslaw Rudowicz, Department of Physics and Materials Science, City University of Hong Kong, 83 Tat Chee Avenue, Kowloon, Hong Kong; 2: 852-2788-7787; FAX: 852-2788-7830; E-mail: apsepr@cityu.edu.hk or Prof. Hiroaki Ohya-Nishiguchi, Yamagata Technopolis Foundation, Institute for Life Support Technology, 2-2-1 Matsuei, Yamagata, 990 Japan; 2: 81-236-47-3132 FAX: 81-236-47-3149; E-mail: ohya@ymgt-techno.or.jp.

## IES Members May Now Use Credit Cards to Pay Dues—

Members may now pay dues by using either a Mastercard or Visa card. By mail, FAX, or E-mail, you may send Chris Felix, U.S. Regional treasurer, the following information: account number, card expiration date, amount you are paying, your name and the year (or years) for which you are paying dues.

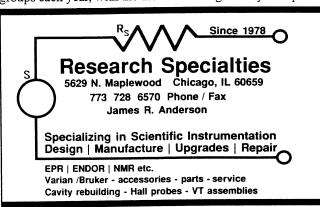
Also, if payment is for more than one person or for someone other than the card holder, be sure to provide all the correct names and each person's dues amount so we can correctly record payments.

Chris Felix, Medical College of Wisconsin, National Biomedical ESR Center; 8701 Watertown Plank Road, Milwaukee, WI 53226, USA; FAX: 1-414-266-8515; E-mail: cfelix@post.its.mcw.edu.

## IES Awards —

#### All 1998 Nominations are Due by Jan. 1, 1998.

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 among the groups each year, with the three following loosely-interpreted



## JEOL USA, Inc.

Manufacturer of CW Electron Spin Resonance Spectrometers Featuring a Compact Design with High Sensitivity and High Reliability

11 Dearborn Road, Peabody, MA 01960, USA Phone: 1-508-535-5900; FAX: 1-508-536-2205 E-mail: dipas@jeol.com

categories: chemistry, physics and instrumentation, and biological sciences (including medicine). These categories are meant to be interpreted very liberally and not to be restrictive.

In 1998, three major awards, the IES Gold Medal, the Bruker Prize, and the Zavoisky Prize will be devoted to the recognition of outstanding achievements in EPR. Prof. Larry Berliner is the continuing Chair of the IES Gold Medal Award Committee.

Gold Medal: Nominations for the 1998 Gold Medal, recognizing benchmark contributions to EPR spectroscopy in Chemistry, should be sent to Prof. Larry Berliner, Chairman of the Gold Medal Committee (e-mail: lberline@magnus.acs.ohio-state.edu) by January 1, 1998.

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 John Pilbrow, George Feher, and Jan Stankowski. For Chemistry - Bruce Gilbert, Chair; N. Hirota, Jim Bolton, and Kev Salikhov. For Biology/Medicine - Harold M. Swartz, Chair; Marjeta Sentjurc, Hideo Utsumi and 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. James R. Norris, Jr.

Fellows of the Society: The IES has created Fellowships to recognize truly outstanding contributions and achievements in electron paramagnetic/spin resonance among distinguished scientists (hopefully, IES members) who are either retired or are close to retirement. See page 1 for 1996 and 1997 Fellows. As the highest international standards are to be applied to the recognition of those worthy of this distinction, their formal connection with the Society will enhance its own image. Nominations for consideration by the Committee are to be sent in confidence by January 1, 1998 to Prof. James R. Norris, Jr., Univ. Chicago, Dept. Chemistry - Searle 133, 5735 S. Ellis Ave., Chicago, IL 60637 USA; 2: 1-773-702-7864; FAX: 1-773-702-0805; e-mail: j\_norris@uchicago.edu.

Publication of the International EPR(ESR) Society

## 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 (richard.cammack@kcl.ac.uk)
Dave Duling (duling@hippo.niehs.nih.gov)

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

In future Computer Corners, we hope to include more installments of Keith Madden's series "Linux on a PC." In the current column, Reef Morse describes freeware for interconversion of EPR data files between several common formats.

#### EPR File Format

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

There are several common formats for EPR data; the BES3T format by Bruker Instruments, the FLS format by Scientific Software Services, and the NIH LMB format implemented by Dave Duling, in order roughly by number of sites. There are other formats as well. The Bruker BES3T format is the most flexible of the three. Data is stored in two files, a parameter file which describes the instrumental parameters to obtain the data and the format of the data in free-form ASCII format. The data itself can be stored in a number of different formats but is most commonly stored as long integer (high-byte first) or 32-bit floating point. Data is stored in files with the same name as the parameter files and a ".spc" extension. For example, "test.par" would be the parameter files for the data file "test.spc". The Scientific Software Services FLS format stores data in ASCII in any format. The information about the type and size of the file

## RESONANCE INSTRUMENTS, INC. is a CONTRIBUTOR to

#### The International EPR Society

EPR spectrometers, components, accessories; Model 8320 Magnet Field Controller for Varian's Mark I & II, others, provides keyboard or computer control; microwave instrumentation to 170 GHz.

### Resonance Instruments, Incorporated

9045 Terminal Drive, Box 1488, Skokie, IL 60077, USA **5**: 1-847-583-1000 FAX: 1-847-583-1021

and the instrumental parameters are stored in ASCII at the beginning of the file. The first line contains a three-letter tag which indicates the nature of the data (multi-dimensional, for example). Dave Duling's software follows the NIH LMB format which has data in floating point format first followed by parameters and comments. For publication-quality output, most data is generally re-cast into a format accessible by a spread-sheet or plotting program. This usually requires the data to be in ASCII format (columns of X-Y data or magnetic field vs. gauss for routine EPR measurements). Thus, there is some utility for software to convert among these various formats.

EWPlot has been written to meet this need. It accepts files in a number of formats, including BES3T, .fls, Dave Duling's (NIH LMB), ASCII, and, by the time you read this, other formats as well. EWPlot allows you to read in and write out data files in these formats, and to plot the data as well. There are a few special features including placement of markers on the spectra, zooming, and simple spectral manipulation. Because EWPlot is changing as other formats are implemented, the manual describing EWPlot's use is slightly behind actual development. However, the salient features of the software are described in detail.

EWPlot is freely available and distributable, although the source code is owned by Scientific Software Services. It may be obtained from the web sites of the Illinois EPR

# Summit Technology Inc.

8827 Osceola Ave.

Morton Grove, IL 60053

Phone: 1-800-735-6327 / 1-847-470-1638

Fax: 1-847-470-1562

Email: 73173.1415@compuserve.com

http://ourworld.compuserve.com/homepages/summit1

## Supporter of the International EPR(ESR) Society

- **♦**EPR Spectrometers
- ♦ Microwave Bridges
- ♦ Magnetic Field Controllers
- ♦ Variable Temperature Controllers
- ◆ Spectrometer Repair and Modification
- ♦ Visit our home page on the world wide web

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

Research Center (http://ierc.scs.uiuc.edu, or by anonymous ftp server at rlb6000.scs.uiuc.edu) and Scientific Software Services (www.scientific-software.com). Both 16-bit (for Windows 3.1) and 32-bit (for Windows 95 and NT) are available.

\*\*\*\*\*

### EPR SPECIALIST VIGNETTES

Edited by Arthur Schweiger

## EPR MONITORING of PLANTS and LICHENS

by Adam Jezierski Faculty of Chemistry, Wroclaw University, 14, Joliot-Curie St., 50383 Wroclaw, Poland fax 48-071-222348

(e-mail: adam@ichuwr.chem.uni.wroc.pl)

and Ewa Bylinska
Institute of Botany, Wroclaw University

#### Introduction

EPR spectroscopy has been proposed as a sensitive and convenient tool for early monitoring of damage of coniferous trees [1]. The results from a two-year screening test in Austrian forests demonstrated the usefulness of this method. There are two types of indication of tree damage detectable by EPR: the intensity of the characteristic six-line spectrum of [Mn(H<sub>2</sub>O)<sub>6</sub>]<sup>2+</sup> complex in conifer needles and the appearance of free-radical signals in the needles. The concentration of the manganese complex seems to be proportional to the overall content of manganese in needles; on the other hand the manganese content has been claimed to correlate with the vitality status of the tree [1]. Thus, the intensity of the EPR signal of the manganese complex correlates with the vitality status. Free radicals observed in damaged needles [1,2] may include ascorbic acid radicals, semiquinone radicals, peroxy radicals, etc. The senescence of cells in biological systems is generally considered to involve free radicals and the radicals responsible for cellular damage are usually short-lived. On the other hand, production of free radicals is intensive in young rapidly developing tissues. In the simple monitoring method of the needles we can observe mainly stable radicals associated with termination of free radical reaction pathways. Some substances in biological systems act as spin traps which form the basis of the EPR approach.

We have observed, however, very strong manganese(II) signals for the needles of weakened and diseased spruces in the Sudety Mountains (south-west Poland); a better correlation between stable radical

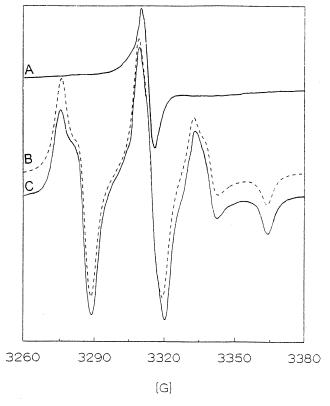


Figure 1. X-Band spectrum of a) typical semiquinone (or similar) free radical (lichen *Umbilicaria polyphylla*); T=295 K; b), c) free radical appearing after action of NO<sub>2</sub> on *Umbilicaria polyphylla*; the signal is characteristic for iminoxy radical RR'C=NO; T=295 K. C - experimental, B - computer simulated spectrum.

signals and vitality status was found in this case [3]. For weakened spruces and pines, radical signals were always detected. Such needles also exhibited iron(III) signals. Action of some harmful chemicals (sulphur dioxide and nitric oxides) on green parts of various plants in the laboratory experiment showed complicated relations between signal intensity of the manganese(II) and stable free radicals signal intensity.

The results are not completely disappointing, but the investigation of conifer needles by EPR spectroscopy seems not to be a simple monitoring method of tree vitality status or air pollution.

We postulate that stable radicals generated in longliving lichens that are extremely sensitive to atmospheric pollution correlate with air pollution, especially sulphur dioxide concentration.

#### Experimental

EPR investigations were carried out on more than 600 samples of lichens from the Sudety Mountains. In this region the average annual concentration of sulphur dioxide is 40 - 80 micrograms/m³, which gives 6-12 Megagrams of sulphur/km² per annum; the local concentrations, however, differ from the above values.

The EPR spectra were recorded at 295 K using an ESP 300E Bruker spectrometer operating at X-band

Publication of the International EPR(ESR) Society

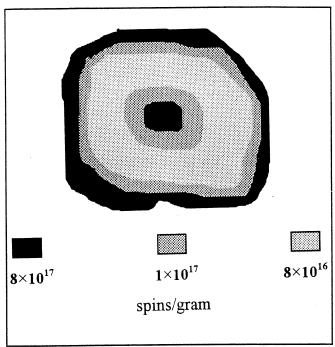


Figure 2. Schematic distribution of semiquinone free radicals in thallus of *Umbilicaria cylindrica*; T = 295 K; the spin concentrations were obtained on the basis of EPR investigations of small fragments of the thallus.

frequencies with a 100 kHz magnetic field modulation. A Li/LiF sample was used for the g parameter calibration; TEMPO, DPPH and ultramarine were used as standards of spin concentration. The quantitative EPR technique was applied (microwave power 20 mW, modulation amplitude 0.2 G, 20.0 mg mass of the sample, standard quartz tubes of the same diameter. etc.). It is characteristic that the stable radical concentration (mainly semiquinone free radicals) is almost identical for the fresh samples and air-dried samples (1- 2 days, 295 K, 70% relative humidity). The concentrations of spins were calculated for dry mass. No change in free radical concentration for samples washed with water is observed.

Representative samples of lichens of the years 1990 to 1996 were collected and investigated. Within this time no significant seasonal alterations of EPR signals could

SCIENTIFIC SOFTWARE SERVICES

P.O. Box 406

Normal, IL 61761-0406 USA Voice/Fax: 309-829-9257

V010071 ux. 000 020 02

Contributor to the International EPR Society

Cost-effective EPR data acquisition, simulation, deconvolution, and imaging software for ALL EPR spectrometers.

Free DEMOs available.

CALL for further information and pricing Web site: http://www.scientific-software.com

be observed (lichens usually are long-lived and slowly-growing organisms).

Representative samples from the following species were used in our EPR investigations: Epiphytes Evernia prunastri, Pseudevernia furfuracea, Parmelia sulcata and Hypogymnia physodes; and species found on granite rocks Umbilicaria cylindrica and Umbilicaria polyphylla.

#### Results

- 1. In all lichen samples broad lines of Fe(III), partially resolved hyperfine lines of Mn(II) species and free radical signals were observed. In these lichens the concentration of free radicals is relatively high (usually  $10^{17}$  to  $10^{18}$  spins/gram). The signal at g between 2.0040 and 2.0044 has complex asymmetric lines; it increases after exposure to sulphur dioxide and decreases after action of some oxidants [3]. The character, reactivity and concentration of the lichen radicals are similar to those observed in humic substances [4,5]. The properties suggest a semiquinone nature of the radicals (Figure 1a).
- 2. Hypogymnia physodes is one of the more common lichens in the south-western part of Poland, and is moderately sensitive to air pollution. We found distinct, statistically confirmed correlations between annual average concentration of sulphur dioxide in the atmosphere and the concentration of stable radicals in the thallus of Hypogymnia physodes. The average concentration of free radicals for the samples from relatively clean areas (no more than 40 micrograms SO<sub>2</sub>  $/ m^3$ ) was about 2.5  $x^{17}10$ spins/g of dry mass, compared to about 6.5 x 10<sup>17</sup> spins/g for polluted areas (80 micrograms  $SO_2/m^3$ ). It is worthwhile to note that local fluctuations of sulphur dioxide concentration (e.g. near small villages, especially located in valleys) may be recognized on the basis of measurements of radical concentration in common Hypogymnia physodes. Similar results were obtained for Umbilicaria cylindrica. These species are found mainly on igneous acid rocks, chiefly in hilly and mountainous regions.

The thallus of the lichen is roughly circular in outline; it is attached to the substrate at a point in the centre of its surface. Thus, the thallus seems to be centrosymmetric. EPR investigations of free radical distribution in the thallus confirmed this suggestion. EPR measurements were carried out on small fragments of the thallus for 25 samples of the lichen. The typical distribution of free radicals in the thallus of *Umbilicaria cylindrica* is shown in Fig.2; the maximum of radical concentration is always in the centre and on the edge. Thus, average samples should be examined in comparison procedure. The characteristic spin concentrations in average samples of *Umbilicaria* 

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

cylindrica collected in relatively clean mountain regions are:  $5.7 \times 10^{17}$  spins/g (distance 100 m from main road),  $4.6 \times 10^{17}$  spins/g (distance 200 m from the same road) and  $4.2 \times 10^{17}$  (distance 300 m).

The above results suggest intensification of the semiquinone (or similar) free radical production in the thallus of lichen in polluted atmosphere. The results are statistically confirmed for more than 600 samples of various lichens; it practically eliminates the role of other environmental factors and accidental agents.

3. We observed the action of NO<sub>2</sub> on some species of Umbilicaria, especially dark-coloured Umbilicaria polyphylla from the Karkonosze (Giant) Mountains (the highest part of the Sudety Mountains) in the laboratory experiment (1% of NO<sub>2</sub> in air, acting 24 h for lichens in closed jar). A new free radical is formed in this case (Fig.1B and 1C). Generation of the radical is observed only for lichens which were grown in relatively polluted places (not far from roads, villages, cottages, etc.); in contrast, the new radical is not observed for samples taken from relatively unpolluted areas.

It is well known that the reaction of NO<sub>2</sub> with carbonyl compounds having a methylene or vinyl group adjacent to the carbonyl leads to the formation of iminoxy radicals, >C=NO type [6]. The spectra obtained in the case of the lichen treated with NO2 are typical for iminoxy radicals:  $g_x = 2.0090$ ,  $g_y = 2.0056$ , g = 2.0028; <sup>14</sup>N hyperfine couplings are:  $A_x = 23.8$  G,  $A_y = 25.6$  G,  $A_z=44.2$  G. It is characteristic that the iminoxy radicals formed in lichen thallus are immobilized; the observed spectra have anisotropic character. In contrast to liquid solutions [6,7] where isotropic spectra have been observed, the anisotropic spectra of iminoxyls can be observed only in some solid matrices, e.g. irradiated solid oximes, zeolite lattices, etc. The observation of an anisotropic spectra in case of lichens at room temperature excludes the possibility of the presence of iminoxyls in the liquid phase.

The formation of iminoxyls during action of  $NO_2$  on Umbilicaria polyphylla which is grown in a relatively polluted place is probably connected with partial degradation of lichenic acids. The acids have acetogenin character; the acetogenins are a large group of natural compounds which owe their formation to a few reactions of the polyacetyl chain  $CH_3$ -CO- $(CH_2CO)_n$ - $CH_2$ -COOH. Oxidative dimerization of acetyl-phloroglucinols creates the widespread lichen product, usnic acid (and possible similar acids). The largest group of acetogenins is represented by the flavonoids. The fundamental degradation procedure of flavonoids, lichenic acids, etc., yields  $\beta$ -diketones. The 1,3-diketones can react with  $NO_2$ ; iminoxyls are formed in this case. The most common lichen substance is usnic

acid; one of the product of degradation of usnic acid is decarbousnic acid with the chain  $-CH_2-CO-CH_2-CO-CH_3$ . It forms **iminoxy** radicals, > C=NO type, in the reaction with nitric dioxide.

4. Perspectives. An area with a characteristic lichen flora that depends on the level and type of air pollution is called a "lichen zone". The standardized lichen zones are well known in several countries. The EPR quantitative measurements of stable radicals in lichens allow one to obtain additional information about air pollution, especially local fluctuations of the pollution. The distribution of the radicals in the thallus (e.g. via imaging procedure) is probably connected with time-dependent aspects of air pollution.

Acknowledgement: Research was supported by KBN, Project 3 T09A 006 11.

#### References:

- Laggner, P., Mandl, R., Schuster, A., Zechner, M., Grill,
   D. (1988) Angew. Chem. Int. Ed. Eng. 27: 1722-1724.
- 2. Stegmann, H.B., Ruff, H.J., Scheffer, K., Knollmuller, M., Loreth, W. (1991) Z. Naturforsch. C: Biosci. 46: 67-70.
- 3. Lisowski, J, Jezierski, A., Bylinska, E. (1993) Appl. Magn. Reson. 5: 15-23.
- 4. Senesi, N. (1992) In: Kubat, J. (Ed) Humus, Its Structure and Role in Agriculture and Environment, pp 11-26, Elsevier Science B.V.
- Drozd, J., Jezierski, A. (1994) In: Senesi, N. and Miano, T. (Eds) Humic Substances in the Global Environment and Implications on Human Health, pp 1119-1124, Elsevier Science B.V.
- Yordanov, N.D., Iliev, V., Shopov, D., Jezierski, A., Jezowska-Trzebiatowska, B. (1982) Inorg. Chim. Acta 60: 9-15.
- 7. Chmielewski, P.J., Jezierski, A., Siatecki, Z. (1992) J. Chem. Soc. Perkin Trans.2: 1421-1424.

### Building the Perfect Beast

by Chris Bender NIH Biotechnology Resource for Pulsed EPR bender@spin.aecom.yu.edu

## OCCASIONAL REFLECTIONS UPON SEVERAL SUBJECTS

I borrowed this issue's title from a book written by Robert Boyle while he was on holiday about 1665. The heady air of Stalbridge perhaps induced Boyle's florid writing style, which, according to literary historians, inspired some of Jonathan Swift's work, including "Gulliver's Travels". The Bronx winter likewise avails itself as an inspirational muse, and so 'The Beast' covers diverse topics.

Publication of the International EPR(ESR) Society

1. Signal Phase in Pulsed EPR. In the past two years I have been at meetings in which papers discussing the phase of the transient EPR signal (echo, FID, etc.) as a source of spectroscopic information have been presented. One of the things that sticks in the back of my mind is the possible systematic error that might occur in these types of experiments. Offhand, I envision problems arising from the traveling wave tube, which is used to amplify the microwave pulse to powers adequate to induce spin dynamics, and the manner in which we generate the microwave pulses to begin The connection between phase variance to the recorded signal lies with the manner in which signals are detected in mixers, both conventional double balanced and quadrature: the DC signal level is a measure of the phase disparity between RF and LO ports. Biphase modulation (or any discrete phase cycling step) will not eliminate random phase errors as would be generated in the following scenarios.

If one works with short (tens of nanosecond) pulses, one generates a low power pulse by modulating the cw output of a reflex klystron or solid state oscillator, and this low power pulse is passed to a traveling wave tube amplifier that is simultaneously turned 'on'. Because of the high voltages required to deflect and control the electron beam, the amplifier cannot be gated on the same time scale as the low power microwave switches and one typically 'turns on' the amplifier for 150 - 200 ns while passing the 10 - 20 ns low power microwave pulse to the tube during this time window. The actual sequence varies with the type of tube one uses tubes tolerant of high duty cycles can be operated with a single 'on' driver pulse into which the entire low power pulse sequence is fit. I think many of us, however, pass a 150 ns amplifier gate for each pulse in the experimental sequence.

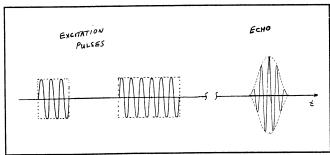


Figure 1.

Ordinarily one positions the low power pulse close to the falling edge of the amplifier gate in order to reduce the spectrometer dead time, and if you are using a video detector to monitor the pulse output of the amplifier, the pulse is considered stable as long as there is no visible amplitude modulation. The fidelity of electron beam control is what determines the quality of the amplified microwave pulse; the ideal being a well focused electron beam that passes through

the helix of the tube. The high voltage pulses that control the beam (swings of about 250 V) determine the beam fidelity, including phase of the slow wave. If the waveform is not consistent, then fidelity may not be retained in the output pulses. Hewlett-Packard markets a very high bandwidth oscilloscope that is called a transition analyzer and measures signals in the phase domain; many of my tests with this analyzer indicate that the pulse phase is very sloppy as the low power pulse is injected near the falling edge of the amplifier gate. This is not surprising because the falling edge of these 250 V pulses are difficult to keep sharp owing

### OXFORD INSTRUMENTS

Supporter of the International EPR Society

#### EPR Cryostats

Cryostats designed specifically for X and Q band EPR experiments

- Helium and nitrogen cooled version available
- Efficient use of cryogen
- Temperature range 1.8 300 K standard (higher temperatures available on request)
- Temperature stability ± 0.1 K

### $Teslatron^H$

Compact high homogeneity Teslatron systems for high field EPR and other applications

- Automated magnetic field and temperature control
- Applied fields from 7 to 20 Tesla
- 10 ppm and 1 ppm homogeneities available
- Integration of experiments using National Instruments LabVIEW<sup>®</sup>
- Available in ultra low-loss cryostats for greatest cryogen efficiency
- Choice of room temperature access or integral variable temperature insert

Call us now for copies of our Teslatron<sup>H</sup> and ESR product guides

Oxford Instruments
Scientific Research Division
Research Instruments
130A Baker Avenue
Concord, MA 01742 USA

Tel: 1-508-369-9933 Fax: 1-508-369-6616 E-mail: epr@oxinst.co.uk



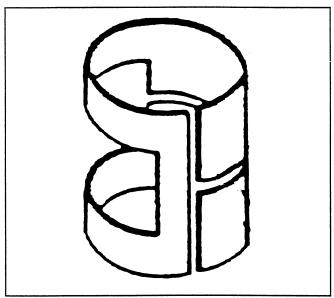


Figure 2

to the capacitive load of the TWT grid (around 200 pf), and so the electron beam is in some unstable state.

Another nagging thought concerning possible phase error concerns the way low power pulses are generated. Again, normally we just gate a cw source such as a reflex klystron, and when you come right down to it, that gating by the diode switch may come at any time during the cycle of the oscillatory waveform. Many of the old Physical Review papers on the subject in which excitation pulse sequences are illustrated are notable because the pulses are all phase-coherent (Figure 1) via some provision within the gating circuit. Similarly, rival NMR gang members occasionally sneer at my spectrometer and ask how I get phase information in my experiments because I do not synchronize my pulses; the volatile situation is defused only when I tell them that I only measure echo amplitudes.

It is possible, albeit tricky, to synchronize the microwave pulses by using NMR instrumental techniques. Basically, one ANDs the delay timing pulse with a clock that is derived from the rf source. For example, a 10 GHz signal has a period of 10<sup>-10</sup> sec. that can be down converted and used as a clock signal to phase lock the source and gating pulse. When he was with our lab several years ago, Subash Gedam built such a device by using a superheterodyne receiver as the down converter and locking device for our switch drivers. A clock impulse with a very sharp leading edge is generated and synchronously triggers (with the leading edge of our programmable delay) an IC that creates a TTL (or preferably ECL) pulse of fixed length that corresponds to the desired pulse length. Subash's circuits relied on a direct interface between sinusoidal waves and the logic family; I later devised a variant that passed a 100 MHz downconverter output to a comb generator whose output yields evenly

spaced 350 ps pulses that work well as a synchronous clock. We were able to demonstrate phase controlled gating of the switch by varying the clock pulse amplitude, but since our lab is concerned only with echoes, the thing never got off the test bench.

- 2. Resonator Variations. Microwave engineering texts from the 1950s and 1960s are a mine of information about design relevant to EPR. Donald King's Measurements at Centimeter Wavelengths (van Nostrand, Toronto 1952) contains a description of a resonator design that provides ample frequency tuning while retaining the same inside diameter. Basically a slot and a gap (Figure 2), one can adjust the resonant frequency by altering the length and width of the gap. You can also make the thing tunable in situ by abutting the gap with a shorting strip that slides along the exterior.
- 3. Nonsinusoidal Carrier. One of the limiting factors of pulsed EPR is insufficient carrier frequency bandwidth for saturating the entire EPR spectral envelope. Jack Freed has successfully used shaped pulses to increase the bandwidth so that it covers many free radicals, but 200 MHz is something of an upper limit with these shaped pulses (see Gorcester et al. in Modern Pulsed and Continuous-Wave Electron Spin Resonance, Bowman & Kevan, eds. Wiley, 1990 pp181ff). As an alternative, there is a body of radar literature that addresses a similar problem by using a nonsinusoidal carrier. In other words, the sinusoidal carrier is passed to a waveshaping network that alters the spectral profile (see any text on spectrum analysis and/or modulation theory). This modified waveform is then gated and amplified. A book devoted to the topic is H. Hartmuth, Nonsinusoidal Waves for Radar and Radio Communication, Academic Press, New York 1981.
- 4. Traveling Wave Tube Amplifier Stuff. I recently overhauled a pair of Space (that's the company name, now known as Quarterwave) 6000 series traveling wave tube amplifiers. The grid pulse-up circuit was modified to resemble some of the faster MOSFET circuits described by Freed (see Gorcester et al., citation above for similar circuit and explanation) and decoupled from the TTL circuits by using optical transmitters & receivers (Hewlett-Packard optoelectronics). When all was said and done, the modulator worked Ok on the bench and behaved as it should according to the manual (1 µs pulses at 1 kHz; the modifications were done by Quarterwave). When sending in a train of short pulses, however, I found myself 'losing' pulses, for example, pulse number 2 in the three-pulse ESEM sequence. To make a long horrible story short, I found that the modified amplifier was not properly impedance matched to the TTL line; a quick remedy entails putting a T-jack on the amplifier input and loading one branch of the Tee with a 50  $\Omega$ termination.

Publication of the International EPR(ESR) Society

I used to have a Hughes 774H 8 - 18 GHz TWT in the thing also. My Hughes tube, however, eventually burned out on me, and since the tube is no longer made, I had to find a replacement. I have gone with Teledyne tubes, but the voltage pulses required exceed the limits arbitrarily set by trim pots on the 6000 series amplifier. As some of you may be aware, the beauty of the Space 6000 is a removable RF drawer that allows you to swap tubes if you have the luxury of several traveling wave tubes that span several octaves. The bad part of the design seems (my impression) to be cheap components used in its manufacture - I have previously reported here that the amp performs much better after replacing all pots with military standard components and the HV jacks with 'real' HV plugs and jacks (as opposed to the \$2 banana jacks one finds in the Newark catalog). Getting back to the Teledyne tubes, one's best bet for modifying the Space amplifier to accept these is by replacing the pots in the drawer, not the HV modulator board in the mainframe. I refer to the paired pots that are screwdriver adjusted within the drawer.

And lastly, the 774H tube spanned two octaves, yet we historically had problems getting good echoes at the high end of K<sub>U</sub> (towards 18 GHz). Numerous theories of this behavior were expounded in this lab over the past 10 years or so ("... <sup>17</sup>O is weird ...", "... it's not at exact cancellation...", etc. etc.). As I replaced the tube, I was forced to reroute some cable to the ferrite isolator that protects the tube from reflections, and it dawned on me that the drawer was outfitted with a WR-90 isolator, which will behave here as a bandpass waveguide filter. Moral of the story: if you buy one of these two octave tubes, make sure you have two isolators with adequate respective bandwidth.

	Failure rate, percent/100 hr				
Lot No.	Time interval, hr				
	0 100	100 500	500 3000	3000 5000	0 5000
1	5	0.25	0.24	0.05	0.26
2	1	0.75	0.36	0.35	0.38
3	5	0.25	0.36	0.40	0.46
4	8	1.25	0.60	0.20	0.64
5	13	3.25	1.2	1.40	1.68

5. Electron Tube Lifetime - Heater Voltage. Regarding klystron and related electron tubes, Jim Anderson wrote a note in this Newsletter about starting up a new klystron at lower than rated heater voltages in order to prolong life. I recently laid my hands on a copy of *Electron Tube Life Factors*, published by McGraw-Hill in 1959 for the US Army Signal Corps. This book documents the

lifetimes of several thousand electron tube devices subjected to various operating conditions. The table above is reproduced from this book and indicates the failure rate of tubes subjected to heater voltages above and below nominal (6.3 V). As already mentioned by Jim, the failure rate is markedly reduced in the initial 100 hours of operation if the voltage is kept slightly lower than nominal; after this period, nominal to slightly lower heater voltages yield comparable failure rates.

### TIPS & TECHNIQUES

### REPLACING VARIAN SPECTROMETER RECORDER CABLES

R. Linn Belford<sup>†,\*</sup> and James P. Wentz\*

†Illinois EPR Research Center
\*School of Chemical Sciences
University of Illinois at Urbana-Champaign

The following question from Roger Lloyd at the University of Memphis recently appeared on the EPR list server: "Where do I get a cable restringing kit for my E-104 (Varian EPR) recorder, that is, the stainless steel cable and especially the little lead anchors?" Rod Claridge of the University of Canterbury, New Zealand, replied that he uses stainless steel fishing line of about the same diameter and



Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

fashions anchors from aluminum rod. He says that the fishing line is a bit stiffer than the original cable, but it works.

For all of our Varian instruments, we have been using another solution for some years with excellent success: We use "wire rope" from McMaster-Carr§ distributors. McMaster-Carr's Catalog # 8930T18 nylon-coated SS 304 (0.019 inch diameter) wire rope really replaces the old Varian cables beautifully, with appropriate flexibility, size, and tensile strength. It's only US\$0.48 per foot in their current catalog in small quantities, and we'd have at least 10 feet of wire rope per axis to be on the safe side. With this wire rope, you don't need any special anchors; we just use figure-8 knots instead of the cable anchors. The figure-8 knot is tied where you want to fasten the wire rope to the spring hook, left loose until you slip the hook through the outside loop, and then snugged up very(!) tightly to grip the hook. Then you just clip off the free end close to the knot and you're in business.

§ McMaster Carr, PO Box 4355, Chicago, IL 60680-4355. Phone 708-833-0300; FAX 708-834-9427.

# AN IMPROVED SIMPLE DEVICE FOR THE PRECISE POSITIONING OF A SAMPLE AT ARBITRARY POINTS OF THE INTRACAVITY SPACE

Milan Mazúr and Harry Morris\*

Department of Physical Chemistry, Faculty of Chemical Technology, Slovak Technical University, Radlinského 9, SK-812 37 Bratislava, Slovakia

\*School of Pharmacy and Chemistry, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK

Incorrect sample positioning in the microwave cavity can cause serious errors in quantitative EPR spectroscopy (see elsewhere [1–8]). Thus, a standard procedure for accurate and reproducable positioning of samples in cavities is useful.

This techniques note describes a modification to our earlier sample alignment tool [9], which allowed precise positioning of cylindrical samples in the TE<sub>102</sub> rectangular cavity but only along the vertical axis, to a new sample setup procedure which allows for precision positioning of cylindrical samples at arbitrary points in the cavity. Like the earlier tool, this new procedure is sufficiently simple and easy to use for routine quantitative EPR experiments.

A diagram is shown in Figure 1, where: (A) is  $TE_{102}$  rectangular cavity, (C) the wave guide from the microwave bridge, (D) the sample access hole, (T) the iris, the point labelled (P) is the centre of the cavity, (E) is a thin-walled quartz tube, (F) is a rod with a calibrated micrometer screw,

(G) is the holder with the matrix screw, (J) is an EPR sample tube, (K) is the connector that connects the sample to the rod (F), (I) are Teflon 'O' rings, which align the sample axis with the axis of the centre of the cavity, (S) is the sample tube of length L, (M) is the upper filling position marker, (R) is the marker for goniometer calibration, (H) is the stopper and marker, which allows realignment of the sample during removal and reinsertion into the cavity. The vertical position, x, of the sample within the cavity can be varied by rotating a calibrated micrometer screw on the rod (F) into the matrix screw holder (G), enabling accurate positioning of the sample within the cavity to better than 0.1 mm. Signal intensities can thus be studied as a function of position,  $\Delta x$ . The final, optimal, sample position can be marked using the stopper/marker (H). Technical details of the movement of line-like samples along the vertical central cavity x-axis were discussed in our previous papers [9-11].

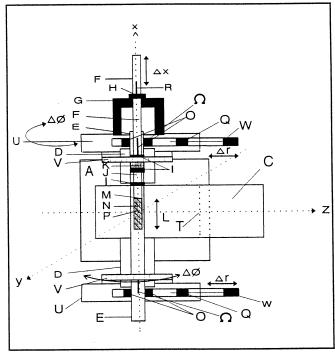
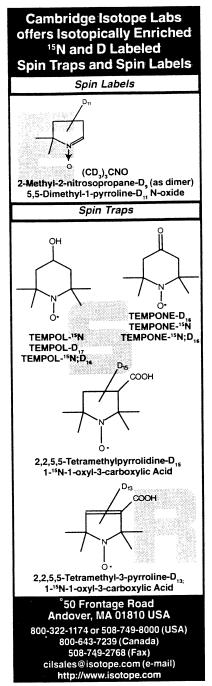


Figure 1. Schematic diagram of the cross section of the single  ${\rm TE_{102}}$  rectangular cavity with the new sample tool for quantitative EPR measurements.

To upgrade the procedure to allow precise positioning of cylindrical samples at any arbitrary point in the cavity, we added the following additional parts: The holder (U), containing the rod (W) with a calibrated micrometer screw, was added on the top and bottom sample access holes (D). To this holder (U) the thin-walled quartz tube (E) was permanently fixed via the connectors (O). The sample assembly parts (F-S) are inserted/removed in/out of the thin-walled tube (E) by the same procedure as is described in our papers [9,10]. The marker and stopper (Q) is for calibrating/fixing the sample in a given orbit with radius, r =

Publication of the International EPR(ESR) Society



 $(y^2 + z^2)^{1/2}$ , in the (y,z) plane. The radius, r, of the orbit in the horizontal plane can be varied by rotating a calibrated micrometer screw on the rod (W) into the matrix screw of the holder (U) which moves the sample tube horizontally across the cavity enabling accurate positioning of sample to better than 0.05 mm. Signal peak-to-peak intensities can be studied as a function of position,  $\Delta r$ . best sample position can be marked using the marker/stopper The top and bottom locking screws (V) with the marker  $(\Omega)$ provide for precise angular orientation —  $[\Phi = \tan^{-1}(y/z)] - and$ permits the operator to start/stop the rotation of the holder (U) with the calibrated angular scale together with thin-walled quartz tube (E) and sample assembly parts (F-S) in the (y,z) plane. These parts rotate around the vertical central axis of cavity, on the circumference of a circle of radius, r. The

angular position,  $\Phi$ , of the sample on this fixed orbit can be varied by rotating the holder (U) with the calibrated angular scale over the marker ( $\Omega$ ) on the locking screw (V), the accuracy is better than 0.5°. The peak-to-peak signal intensities can be studied as a function of position,  $\Delta\Phi$ . The final, optimal, sample position can be fixed with the locking screw (V).

In summary:  $\Delta x$  represents the freedom of vertical sample tube movement along an arbitrary axis parallel to the vertical central x-axis of the cavity.  $\Delta r$  represents the freedom of horizontal movement of the sample tube in the

arbitrary horizontal (y,z) plane, which is perpendicular to the vertical central x-axis of the cavity, and for which the vertical coordinate is x.  $\Delta\Phi$  represents a freedom of the horizontal rotation of the sample tube in the arbitrary horizontal (y,z) plane on the orbit with the fixed radius, r. The centre of this rotation is situated on the vertical central x-axis of the cavity. The variation of the signal peak-to-peak intensities can thus be studied as a function of the sample movement along the three independent r-,  $\Phi$ - and x- axes.

In conclusion, implementing a new simple modification to the sample insertion procedure for the Bruker  $TE_{102}$  cavity as described above significantly increases the accuracy to which quantitative EPR measurements can be made. The adaptation can be used with the double  $TE_{104}$  cavity without modification (see ref. 12), and with the cylindrical (e.g.  $TE_{011}$ ) and other manufacturer (e.g. Varian) cavities with minor modifications.

#### References

- M. Sueki, G.A. Rinard, S.S. Eaton, and G.R. Eaton, J. Magn. Reson., Ser. A, 118 (1996) 173.
- 2. N.D. Yordanov, Appl. Magn. Reson., 6 (1994) 241.
- 3. V. Nagy, Appl. Magn. Reson., 6 (1994) 259.
- 4. R.C. Barklie and L. Sealy, J. Magn. Reson., 97 (1992) 611.
- V.J. Nagy and J. Plaček, Fresenius J. Anal. Chem., 343 (1992) 863.
- 6. S.S. Eaton and G.R. Eaton, Anal. Chem., 49 (1977) 1277.
- 7. G. Casteleijn, J.J. ten Bosch and J. Smidt, J. Appl. Phys., 39 (1968) 4375.
- 8. C.P. Poole, Electron spin resonance. A comprehensive treatise on experimental techniques, Wiley-Interscience, New York, 1967.
- 9. M. Mazúr and H. Morris, EPR Newsletter, 8 (1996) 10.
- 10. M. Mazúr, M. Valko, R. Klement and H. Morris, Anal Chim. Acta. 333 (1996) 249.
- M. Mazúr, M. Valko, H. Morris and R. Klement, Anal. Chim. Acta, 333 (1996) 253.
- 12. M. Mazúr, M. Valko, R. Klement and H. Morris, Rev. Sci. Instrum., in press, 1997.

### **CONFERENCE REPORTS**

#### FIRST ASIA-PACIFIC EPR/ESR SYMPOSIUM

The First Asia-Pacific EPR/ESR Symposium was held from January 20 through 24 at the City University of Hong Kong. The symposium was attended by about 140 participants from 22 different countries, among whom 110 were from the Asia-Pacific, Europe and North America whereas 30 were from Hong Kong, mainland China and Taiwan. There were 8 invited plenary lectures, 3 invited plenary talks, 114 oral presentations, and 69 poster

### AMERICAN INSTITUTE OFPHYSICS

**Professional Societies & Publications** 

500 Sunnyside Boulevard Woodbury, NY 11797-2999 USA Phone: 1-516-576-2411 Fax: 1-516-576-2481

presentations, comprising together 183 presentations. The opening ceremony was officiated by Prof. H.K. Chang, the President of City U.

The meeting featured the following plenary lectures: Prof. S.H. Choh, Republic of Korea: EPR Study of paramagnetic defects in LiNbO3 single crystals; Prof. Richard Cammack, UK: Bio-medical applications of EPR spectroscopy; Prof. C.A.J. Ammerlaan, The Netherlands: Magnetic Resonance Spectroscopy of rare-earth doped semiconductors; Prof. J.M. Spaeth, Germany: Electrical detection of EPR and ENDOR: New possibilities for the study of defects in semiconductors; Prof. John R. Pilbrow, Australia: Pulsed and CW EPR in materials science; Dr. Richard Bramley, Australia: EPR meeting the challenges of new materials; Prof. M. Ikeya, Japan: New applications of electron spin resonance - dating, dosimetry and microscopy; Prof. Noboru Hirota, Japan: Chemically induced dynamic electron polarization (CIDEP) studies of photochemical reactions at different magnetic fields; and plenary talks: Prof. Mitsuhiro Motokawa, Japan: Submillimeter wave ESR of magnetic materials in high magnetic fields; Prof. Yves Servant, France: EPR studies of spin transitions: A review; Prof. A. Romanyukha, Russia: Comparative study of different EPR materials for use in clinical dosimetry.

The interdisciplinary character of the EPR/ESR spectroscopy was reflected in the scientific programme, which consisted of the plenary sessions and four parallel sessions: (1) biology, life and medical sciences, (2) chemistry, earth and environmental sciences, (3) physics

and materials science, (4) new developments and cross-disciplinary areas. The refereed proceedings will be published in a book, "Modern Applications of EPR/ESR: From Biophysics to Materials Science", by Springer-Verlag, Singapore.

The symposium provided opportunities for specialists in many different fields to interact. We were fortunate that many distinguished scientists had joined the symposium. The symposium provided also an opportunity to bring the state-of-the-art knowledge of EPR to Hong Kong and southern China. An exhibition of EPR/ESR instrumentation as well as of scientific journals and books by Springer was held during the symposium. The social programme was comprised of Sunday evening's welcoming mixer, Monday evening's reception, and Thursday evening's symposium banquet.

The symposium was a great success, judging by the positive feedback received from many participants. Moreover, the Asia-Pacific participants gathered at the inaugural meeting of the Asia-Pacific EPR/ESR Society (see details in Society Affairs) unanimously voted a proposal that the second Asia-Pacific EPR/ESR Symposium be held, not in another country as suggested by the LOC Chairman, but again at City U. in Hong Kong in 1999. However, organisation of the next symposium would require significant University resources, which the University does not feel able to muster again so soon. Therefore, efforts will be made to find alternative arrangements for the second Symposium. As president of the Asia-Pacific EPR/ESR Society, I will try to convince researchers from other institutions within the Asia-Pacific region to organise and host the symposium. Perhaps we should follow the pattern of the European Federation of EPR Groups. The European EPR Symposium is to be organised every three years in a different country with a national EPR group in charge of the local organization being also responsible for handling the financial affairs.

On behalf of the Local and International Organizing Committee I would like to thank the organisations who financially supported the symposium, namely, Lee Hysan Foundation, The Croucher Foundation and Beijing - Hong Kong Academic Exchange Centre.

# CPI Sets the Standard for EPR Klystrons The plot illustrated was taken with a Varian weak pitch sample in a

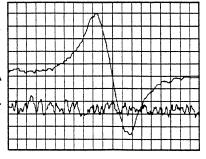
CPI Replacement Klystrons deliver:

- Optimum application flexibility Long Life
- Reliable performance, low noise New warranty
- X band for Century Series, E lines, plus Q band Now available directly from CPI. For more information call CPI at 1-800-843-8780 or 415-846-3188 from outside the U.S.



formerly a division of Varian®

taken with a Varian weak pitch sample in a TE102 cavity under the conditions specified in the Varian E-line series unmodified (E-102/E-109 bridge) instruction manual. Signal to noise ratio represented is 245:1. A 2.8 conversion factor was used to convert rms noise to P-P noise. The weak pitch sample had a .683 multiplication factor. Without the multiplication factor, the signal to noise would be 359:1.



Publication of the International EPR(ESR) Society

This was the first international conference that our local team and I have organised. The administrative and printing costs were kept to a minimum. We did not hire a professional conference organiser. Instead, we provided as many travel and accommodation grants to our colleagues in need as possible and waived the registration fee for about 40% of the participants. We were helped in this regard by the caring attitude of our invited speakers who opted for standard accommodation instead of an upper class hotel. This symposium may be compared to a "home-made cake." Thank you to all who have helped to successfully "bake the cake," especially the hard working colleagues from the Local Organizing Committee.

Czeslaw Rudowicz Chairman of the Local and International Organizing Committee

### **BOOKS & PROCEEDINGS**

<u>SPIN LABELING: THEORY AND APPLICATIONS</u> (Lawrence J. Berliner, Ed.): Reprinted copies of Volumes I and II available.

While Prof. Berliner still gets frequent inquiries about how to obtain the first two volumes, the Academic Press has declared them out of print two years ago. No more copies exist for sale (at least to his knowledge). Amazingly, these volumes are still quite useful. Volume I is somewhat of a classic and has become a 'textbook'.

Academic Press has released the copyrights and rights to reproduce the books to Prof. Berliner. The Illinois EPR Research Center, as part of its service to the EPR community, will run off and distribute an initial batch of copies with a durable hard binding. The cost to you will be very much lower than the publisher's most recent prices.

How many people are <u>seriously</u> interested? Please e-mail or FAX Becky Gallivan at the IERC (ierc@uiuc.edu or 217-333-8868; full address in masthead at the end of this Newsletter). We will respond to you with details of exact cost and the estimated run/shipping date. Please state your interest in Vol. I, II or both: SPIN LABELING: THEORY AND APPLICATIONS (Vol I), Academic Press (1976), 592

pages. SPIN LABELING: THEORY AND APPLICATIONS (Vol II), Academic Press (1979), 360 pages.

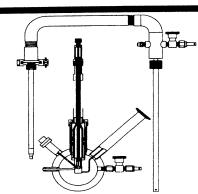
Larry Berliner, Linn Belford, Bob Clarkson

# NMR OF PARAMAGNETIC SUBSTANCES, by Ivano Bertini and Claudio Luchinat.

This, the latest book originating from the Florence magnetic resonance centre, has appeared in 1996, printed in the Netherlands by Elsevier as a ca. 300-page volume. The EPR community may well find it of interest, for one since the authors make a special tutorial effort to deal with spin-density delocalization and contact/pseudo-contact shifts, as well as chemical exchange. The book appears as Volume 150 of Coordination Chemistry Reviews, from which fact it may be correctly deduced that there is considerable emphasis on metal-ion complex phenomena.

This treatise begins at an elementary level, dealing generally with spins, magnetic moments, susceptibility and resonance. There is adequate coverage throughout of the mathematical necessities, with few in-text derivations (but see Appendices II-IV) and without any special claim to be sophisticated or elegant. All equations use SI units. This nit-picking reviewer would have preferred to see more care taken in use of the word 'tensor' (e.g., p.12 for g), in making more clear what quantities are vectors and which are scalars (e.g., p.26 for  $\mathbf{B}_1$ ), and generally in the use/non-use of hyphens. However, the English in grammar and vocabulary is of high quality. The volume is well illustrated, and appears to contain few typos. The somewhat gossameric quality of the paper used for the book is ameliorated by the affordable price of the volume.

Chapter 2 - The Hyperfine Shift - discusses the basics, treats "metal"-centered and ligand-centered contributions, and covers the latter topic with various examples using typical nitrogenic ligands. Lanthanides and actinides, used as shift reagents, are also treated. A subsequent chapter, 6, deals with and summarizes the relevant electronic and nuclear relaxation phenomena, and a later chapter ties in the nuclear Overhauser effect on nuclear relaxation. Chapter 7 is important in that it portrays the two-dimensional spectroscopic developments of



#### EPR/ENDOR CRYOSTATS

Complete Systems - Fastest Cooldown - Lowest Temperatures
Uses liquid helium or nitrogen - Push or Pull Operation
Plus, our replacement transfer line for your existing cryostat can Save you up to 50% on your liquid helium costs - Cool down samples faster Lower your terminal temperature and increase reliability!
Call or fax us for additional information:

**CRYO** Industries of America, Inc. 11 Industrial Way, Atkinson, NH 03811 Tel: (603) 893-2060; Fax: (603) 893-5278

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

the last two decades; that should be useful to the EPR spectroscopists. Various "multi-metallic" systems (e.g., Fe, Co, Ni) are discussed at some length, as are certain high-resolution solid-state examples in Chapter 8.

While noting that no claim for complete literature citation was made, some omissions are regretted by this reviewer: No reference to the major review article on nuclear spin relaxation in paramagnetic systems [J. Kowalewski et al., Progr. NMR Spectrosc. 17, 141 (1985)], no mention of paramagnetic metalion complexes as relaxation agents for NMR imaging [see R.B. Lauffer, Chem. Rev. 87, 901 (1987)], no retrospective to the original work on lanthanide shift reagents [C.C. Hinckley, J. Am. Chem. Soc. 91, 5160 (1969)].

The present book joins its illustrious 1973 predecessor, "NMR of Paramagnetic Molecules" (edited by G.N. La Mar, D. DeW. Horrocks Jr., and R.H. Holm), in presenting basic concepts, and of course adds a summary of major new developments in techniques, technology and data now in the literature - including some 1996 references. It is a worthwhile and welcome addition to our libraries. This reviewer enjoyed reading this volume, and learned considerably from it.

John A. Weil, Professor Emeritus of Chemistry University of Saskatchewan, Saskatoon, Canada

### **NOTICES OF MEETINGS**

### TWENTIETH INTERNATIONAL EPR SYMPOSIUM at the 39th Annual Rocky Mountain Conference, August 3-7, 1997, Denver, CO, USA.

The EPR Symposium will start Sunday evening with an open house at the University of Denver EPR labs, including refreshments provided by Bruker Instruments.

In this Symposium we will emphasize different ways of looking at unpaired electron spins and the complementary information that can be obtained by different techniques. The "normal" CW experiment is most widely used, but it is not necessarily the most powerful way to answer a particular question. There are many other methods including various multiple resonance and time-domain techniques. Since this will be the 20th year for the EPR Symposium we hope to have at least 20 techniques represented.

The preliminary program for the 1997 EPR Symposium can be viewed at:

#### http://www.du.edu/~seaton/eprsym.html

Additional information will be posted on this web site as it becomes available, or contact: Prof. Sandra S. Eaton or Prof. Gareth R. Eaton, Dept. of Chemistry and Biochemistry, Univ. of Denver, Denver, CO, 80208-2436, USA. 2: 303-871-3102; FAX: 303-871-2254; E-mail: seaton@du.edu.

### THIRD EUROPEAN ESR MEETING, August 25-29, 1997, Leipzig, Germany.

The title of this meeting is "Modern Aspects of Structure and Dynamic Investigations of Paramagnetic Systems by EPR". A list of topics for this meeting can be found in the EPR Newsletter, Vol. 7 No. 4.

Scope of the Meeting: This series of ESR meetings was initiated in 1991 in Padua by the Italian and UK ESR groups and continued successfully in Paris in 1994. The meeting in Paris collected more than 180 ESR spectroscopists from six European countries. This 3rd ESR meeting intends to bring together the European ESR spectroscopists from all fields of application of this powerful spectroscopy to a fruitful and exciting discussion.

Presently the European Federation of ESR Groups encloses the ESR Group of the Royal Society of Chemistry, the Gruppo Italiano di Risonanza di Spin Elettronico, the Benelux EPR Discussie Groep, the Polish ESR Group, the Groupe d' Application de la RPE, the Russian ESR Group, and the German ESR Discussion Group. The International EPR Society is included in the preparation of the scientific programme to present the IES prize winners for 1997 with their prize lectures.

Scientific Committee: M. Brustolon (Padua), N.D. Yordanov (Sofia), C.J. Rhodes (Liverpool), B. Catoire (Paris), C.C. Rowlands (Cardiff), P. Devaux (Paris), A. Alberti (Bologna), K. Salikhov (Kazan), A.J. Hoff (Leiden), H. Kurreck (Berlin), P. Gast (Leiden), R. Böttcher (Leipzig), H.B. Ambroz (Warszawa), D. Beckert (Leipzig), A. Jezierski (Wroclaw).

Organizing Committee: D. Beckert (Leipzig), G. Völkel (Leipzig), R. Böttcher (Leipzig), A. Pöppl (Leipzig), D. Michel (Leipzig), L. Kießling (Frankfurt/Main).

Scientific Programme: Monday, August 25, 1997—Opening Session (Chairman: M. Brustolon, Padua, Italy); High-Field/High-Frequency EPR and ENDOR on Radicals and Radical Pairs in Photosynthesis: Structure and Dynamics (K. Möbius, Berlin, Germany); Site-selective Isotope Substitution as a Tool to Unravel by Multifrequency EPR and ESEEM the Binding of Cofactors in Photosynthetic Reaction Center (A. Hoff, Leiden, The Netherlands); Exploiting Quantum Beats with Time Domain EPR (J. Norris, Chicago, USA); Study of Liquid Phase Photo-Induced Reactions with Fourier Transform EPR (K.-P. Dinse, Darmstadt, Germany); Quantitative Time-Resolved EPR CIDEP Investigations after Laser Flash Photolysis of Azoalkanes in Solution (H. Paul, Zürich, Switzerland); Analytical Description of Electron-Electron-Nuclear Three-Spin Mixing in Spin-Correlated Radical Pairs (G. Jeschke, Bonn, Germany). Pulsed Electron Magnetic Resonance of Transition Metal Ions in Mesoporous MCM-41 Materials (L. Kevan, Houston, USA); The Matrix Effect in EPR Spectroscopy of Aryl Cations of Strong Dipolar Interaction (H. B. Ambroz, Warsaw, Poland); Kinetics of Electron Self-Exchange Reactions Measured by EPR Spectroscopy and the Application of Marcus Theory (G. Grampp, Graz, Austria); The

Publication of the International EPR(ESR) Society

Determination of Bond Dissociation Energies by EPR (G. F. Pedulli, Bologna, Italy). Tuesday, August 26, 1997-New Concepts in Pulse EPR Spectroscopy (A. Schweiger, Zürich, Switzerland); Radiofrequency ESR Imaging and Spectroscopy (D. G. Gillies, Surrey, UK); EPR and Magic-Angle Spinning (M. Hubrich, Mainz, Germany); Nature, Structure and Physicochemical Properties of Electron-rich Surfaces (E. Giamello, Turin, Italy); Paramagnetic Silver Clusters in Molecular Sieves (J. Michalik, Warsaw, Poland); Comparative Study of Hole Processes on Dye Molecules for Spectrally Sentisized AgBr and AgCl Microcrystals (T. Ceulemans, Antwerpen, Belgium); Electronic Structure and Protein Interactions of Radical Ions and Triplet States in Photosynthesis Studied by CW- and Pulsed EPR/ENDOR (F. Lendzian, Berlin, Germany); ESEEM and HYSCORE of VO2+ in Biological Systems (J.- L. Zimmermann, Gif-sur-Yvette, France); Cross-Regulation of Metalloenzymes, Triggered by Nitric Oxide: An Overview (Y. Henry, Orsay, France); ESR and Iron in Biological Systems (M. Symons, Leicester, UK). Wednesday, August 27, 1997-Presentation of the International ESR Society Awards (J. Norris, Chicago, USA); Lectures of the IES Award Prize Winners (N. N.); Excursion to Dresden. Thursday, August 28, 1997—Pulsed EPR Spectroscopy at 95 GHz: Technology and Applications (J. Schmidt, Leiden, The Netherlands); Structure-Mobility Relations as Studied by High-Field EPR (A. Dubinskii, Moscow, Russia); Investigation of Fullerenes by 2-mm (V.I. Krichnichyi, EPRSpectroscopy Waveband Chernogolovka, Russia); Librations of Radicals as Studied by EPR and ESE (Yu.D. Tsvetkov, Novosibirsk, Russia); Molecular Dynamics of Radicals in Solid Phases (U. Segre, Modena, Italy); Shallow Donors in Semiconductors W-Band Double Resonance Spectroscopy (G. Denninger, Stuttgart, Germany); Nature, Structure and Physico-chemical Properties of EPR, ENDOR and ESEEM in Single Crystals of (4Fe-4S) Clusters, Models of Active Sites of FeS-Proteines (B. Lamotte, Grenoble, France); New Generation of Alanine/EPR Dosimeters (V. Gancheva, Sofia, Bulgaria); ESR Study of DNA Synthesis System: the Mechanism of DNA Damage, Repair and Protection (K. Pulatova, Moscow, Russia); The Electronic Structure of the Blue-Copper Site. A Pulsed High-Frequency EPR Study (M. van Gastel, Leiden, The Netherlands); Hyperfine Tensors for  $I = \frac{1}{2}$  Nuclei by Contour Lineshape Analysis. Application to Inorganic Complexes and Protein Active Sites (S. A. Dikanov, Novosibirsk, Russia); Analysis of Cross Peak Lineshapes in Proton and Deuterium HYSCORE Spectra in Disordered Systems (A. Pöppl, Leipzig, Germany); Explicit Analytical Formulae for the ESEEM Arising from Hyperfine Coupling to Nuclei of Arbitrary Spin (A. Ponti, Milano, Italy); ESR Spectra at 75 GHz by Using a Whispering Gallery Mode (WGM) Dielectric Resonator and an Electromagnet (A. Colligiani, Napoli, Italy). Friday, August 29, 1997-Application of EPR to Bioinorganic Systems (R. Cammack, London, UK); <sup>31</sup>P Labelled Nitroxides and Nitrones (P. Tordo, Marsielle, France); EPR and ENDOR at Frequencies above 200 GHz (H.

van Tol, Grenoble, France); Electron Spin Relaxation in Crystals with Jahn-Teller Effect (S. Hoffmann, Poznan, Poland); High Resolution EPR Investigations of the Proton Order in the Proton Glass Betainephosphate/Phosphite (G. Völkel, Leipzig, Germany); Paramagnetic Properties of Endohedral Fullerenes (A. Bartl, Dresden, Germany).

Location: The meeting will be held at the University of Leipzig, Augustusplatz, which is situated in the centre of the city.

Accommodation: The agency Dr. Augustin Studienreisen, Leipzig, is entrusted with the reservation of hotel rooms. Dr. Augustin Studienreisen GmbH, Könneritzstr. 73, D-04229 Leipzig, Germany; 2: 49-341-48458-0; FAX: 49-341-48458-29. The Congress hotel is the Mercure Hotel Leipzig, situated opposite the University. Prices per night per room including breakfast, service and taxes are: DM 180,- double occupancy, DM 125.- single occupancy. Application for hotel accommodation should be made before June 24, 1997. The customers will be held accountable for non-occupancy of reserved rooms.

The check-in facilities, cashier's counter, information desk, boards for messages and announcements etc. are located on the ground floor of the lecture halls building. The office will be open as follows: Sunday, August 24: 17.00 - 19.00 h; Monday, August 25: 08.00 - 17.00 h; Tuesday, August 26: 08.00 - 16.00 h; Wednesday, August 27: 08.00 - 12.00 h; Thursday, August 28: 08.00 - 16.00 h; Friday, August 29: 08.00 - 12.00 h. \$\mathbb{\sigma}\$: 49-341-9731-113; FAX: 49-341-9731-149.

Congress Language. The official language of the Meeting will be English. There will be no translation facilities.

Lunch. The University Cafeteria "Mensa" as well as the Hotel Mercure (located at Augustusplatz opposite the lecture halls building) will provide lunch during the Meeting (to be paid individually, not included in the registration fee).

Travel Agent. For reservation and booking of any transport or hotel please inquire at the counter of Dr. Augustin Studienreisen.

For more information, contact DP Dr. Habil. Dieter Beckert, Max-Planck-Society, Research Unit "Time Resolved Spectroscopy" at University Leipzig, Permoserstr. 15, D-04303 Leipzig, Germany; 2: 49-341-235-2630; FAX: 49-341-235-2317; E-Mail: beckert@mpgag.uni-leipzig.de. Or access our web site at: http://www.uni-leipzig.de (keywords: Veranstaltungen, Tagungen).

# 7th EUROPEAN CONFERENCE on the SPECTROSCOPY of BIOLOGICAL MOLECULES (ESCBM), September 7-12, 1997, San Lorenzo de El Escorial, Madrid, Spain.

This major International Conference will focus on the structure and dynamics of biological molecules and related systems as revealed by Raman and infrared spectroscopies and other methods, particularly NMR, CD, optical absorption and fluorescence, inelastic neutron scattering, X-ray

crystallography, computer graphics and molecular mechanics and dynamics. The Conference offers the opportunity to unite spectroscopists and specialists of Biochemistry, Medicine and Biology interested in the application of spectroscopic methods for life science research. The conference is sponsored by Comité Español de Espectrascopía (SEDO) and Universidad S. Pablo - CEU.

Please direct all correspondence to the Conference Chairman: Dr. P. Carmona, ECSBM'97 Chairman, Instituto de Estructura de la Materia (CSIC), Serrano 121, 28006 Madrid, Spain; **\***: 34-1-5616800; FAX: 34-1-5645557; E-mail: pcarmona@pinar1.csic.es; Internet web page:

http://www.uned.es/convoca/ecsbm97.htm.

RUSSIAN ACADEMY of SCIENCES DIVISION of GENERAL and TECHNICAL CHEMISTRY, UNITED INSTITUTE of CHEMICAL PHYSICS, RUSSIAN FOUNDATION for BASIC RESEARCH, 40 YEARS of FREE RADICALS ESR STUDIES, 5th Conference: "Physics and Chemistry of Elementary Chemical Processes," (In memory of Professor Vladislav V. Voevodskii), September 29th-October 3rd, 1997, Chernogolovka, Russia.

You are cordially invited to participate in the work of the 5th All-Russia Conference on Physics and Chemistry of Elementary Chemical Processes dedicated to the memory of Professor Vladislav V. Voevodskii (Academician) and honoring the 80th annivesary of his birth. The Conference will be held (29.09.97-3.10.97) by the Institute of Chemical Physics in Chemogolovka, an Academic Town of the Russian Academy of Sciences, located 50 km away from Moscow. Both foreign and national participants are invited. Official languages of the Conference are Russian and English.

Organizers of the Conference: Institute of Chemical Physics in Chernogolovka, RAS; Semenov Institute of Chemical Physics, RAS; Emanuel Institute of Biochemical Physics, RAS; Centre of Photochemistry, RAS; Institute of Energy Problems of Chemical Physics, RAS; Institute of Structural Macrokinetics, RAS; Institute of Chemical Kinetics and Combustion, Siberian Division, RAS; Boreskov Institute of Catalysis, Siberian Division, RAS; International Centre of Tomography, Siberian Division, RAS; Moscow Institute of Physics and Technology.

Conferences in the memory of Prof. V. Voevodskii are organized every five years in turn by Moscow and Novosibirsk and are devoted to the currently basic problems of physics and chemistry of elementary chemical processes. The forthcoming 5th Conference will deal with the problems and prospects of ESR spectroscopy of free-radical processes - the field of science whose foundation was laid by Prof. V. Voevodskii and his pupils, among them Professors K. Zamaraev and Ya. Lebedev prematurely deceased in 1996. The first Voevodskii Prize will be awarded at this conference (see *IES Affairs* in this issue for details).

Main scientific topics: ● kinetics and dynamics of elementary chemical processes, electron transport, weak interactions, effects of surrounding, ● free radicals in liquid, gas and on the surface; chain and catalytic reactions, ● free radicals in solids, synthetic and natural polymers, ● free radicals in high-energy chemical reactions (photo-, radiation, plasmo- and mechanochemistry), ● free radicals in ecology, biology and medicine, molecular dynamics, spin lables and traps, ● new approaches and methods in ESR spectroscopy.

Organizing Committee: V.I. Goldansky (Chairman), Yu.D. Tsvetkov (Vice Chairman), C.M. Baturin (Vice Chairman), A.I. Mikhailov (Secretary).

Scientific Advisory Board: M.V. Alfimov, S.M. Aldoshin, A.A. Berlin, L.A. Blumenfeld, A.L. Buchachenko, F.I. Dubovitskii, V.E. Fortov, V.A. Kabanov, M.I. Kabachnik, V.B. Kazanskii, N.V. Karlov, S.N. Khadzhiev, N.N. Kudryavtsev, V.V. Lunin, G.B. Manelis, A.A. Mantashyan, A.G. Merzhanov, Yu.N. Molin, O.M. Nefedov, V.N. Parmon, A.K. Pikaev, R.Z. Sagdeev, K.M. Salikhov, A.E. Shilov, V.L. Talroze.

Programme Committee: Chairman - P.Yu. Butyagin; V.V. Azatyan, I.M. Barkalov, P.P. Barashev, G.N. Bogdanov, N.N. Bubnov, L.T. Bugaenko, A.A. Dubinskii, E.B. Gordon, S.N. Kabakchi, A.I. Kokorin, A.V. Kulikov, M.Ya. Melnikov, V.P. Melnikov, V.K. Milinchuk, M.K. Pulatova, A.P. Purmal, O.M. Sarkisov, V.A. Smirnov, S.M. Solodovnikov, L.N. Stesik, A.F. Vanin, A.V. Vannikov, A.M. Vasserman, A.A. Yudanov.

Registration Fee. The registration fee (450USD) includes the living in the house-rooms, breakfast, lunch, dinner, coffee breaks and the book of proceedings). Cash payment during registration for the Conference.

Visa Information. Each participant (and accompanying person) should submit to the Organizing Committee the following information: full name, sex, date and place of birth, citizenship, name and address of the participant's institution, home address, passport number, dates of issue and expiration, location of the suitable Russian Consulate Office.

Abstracts and all correspondence should be addressed to Prof. Alfa Mikhailov, Institute of Chemical Physics RAS, Chernogolovka, Moscow Region, 142432, Russia. E-mail: esrconf@icp.ac.ru. Information about the Conference can also be found on the Conference's WWW home page:

http://www.icp.ac.ru/Conference/ESR97/eindex.html.

More urgent information could be obtained from Dr. Maryana V. Voevodskaya, **3**: 7-095-9385151, FAX: 7-095-9381838.

SECOND INTERNATIONAL CONFERENCE on BIORADICALS and FIFTH INTERNATIONAL WORKSHOP on ESR(EPR) IMAGING AND *IN VIVO* ESR SPECTROSCOPY, October 12-16, 1997, Yamagata, Japan.

The conference will treat all aspects of bioradicals, with special attention to ESR spectroscopy. The following subjects comprise the main scientific scope:

Publication of the International EPR(ESR) Society

- A-1. Chemistry and Biochemistry of Bioradicals;
- A-2. Metalloproteins
- A-3. Pathophysiology
- A-4. Nitric Oxide NO
- A-5. Antioxidants and Food Science
- A-6. Redox regulation and Signal Transduction
- B-1. ESR Imaging and in vivo ESR
- B-2. Biological applications of ESR New ESR Technologies.
  - C. Other topics

Correspondence: ICB II Secretary General - Dr. Hiroaki Ohya-Nishiguchi, Institute for Life Support Technology, Yamagata Technopolis Foundation, 2-2-1 Matsuie, Yamagata 990, Japan; ₹: 81-236-47-3134; FAX: +81-236-47-3149;

E-mail: ohya@ymgt-techno.or.jp.

FOR A SCHEDULE OF INVITED LECTURES, LOOK AT THE EPR NEWSLETTER WEB PAGE -- http://ierc.scs.uiuc.edu/news.html

### FIFTH INTERNATIONAL CONFERENCE ON SPIN CHEMISTRY, October 26-31, 1997, Jerusalem, Israel.

For official circular and information please contact Haim Levanon, Dept. Physical Chemistry, The Hebrew University, Jerusalem, 91904 ISRAEL. **2**: 972-2-658-5544; FAX: 972-2-618-033; E-mail: levanon@vms.huji.ac.il. <u>Visit the conference web page for more complete information about this meeting:</u>

#### http://chem.ch.huji.ac.il/farkas/intra meet.html

# 29th SOUTHEASTERN MAGNETIC RESONANCE CONFERENCE, October 30-November 1, 1997, Gainesville, Florida.

The 29th meeting of the Southeastern Magnetic Resonance Conference (SEMRC) will be held October 30 to November 1, 1997 in Gainesville, Florida, on the campus of the University of Florida. The SEMRC brings together investigators, students and vendors with interest in NMR, EPR and ICR.

The conference will feature invited and contributed papers and posters in NMR, MRI, EPR and ICR; including time-resolved and multidimensional spectroscopies, high magnetic fields and applications in materials sciences, physics, chemistry, biology and the medical fields. Invited keynote speakers are: Michael Mehring (Univ. Stuttgart), Hans Thomann (Exxon Corp.) and Warren Warren (Princeton Univ.).

Submission of Abstracts. Abstracts are requested for all invited and contributed presentations including posters. Abstracts are due no later than September 15, 1997. They will be reproduced and bound for distribution to participants.

Registration. The advance registration fee is \$45 for regular attendees, \$25 for postdoctoral fellows and graduate students, and \$25 for companion registration. The deadline for advance registration is September 15, 1997. After that date, registration fees will be \$60 for regular attendees, \$40 for postdocs, graduate students and compansions and \$15 for undergraduate students.

For more information, contact Lori Clark, Univ. Florida, Dept. Chemistry, Box 117200, Gainesville, FL 32611-7200, USA; **3**: 1-352-392-4654; FAX: 1-352-392-0872; E-mail: lori@chem.ufl.edu.

# ANZMAG 97, 10th AUSTRALIAN MAGNETIC RESONANCE CONFERENCE, December 7-10, 1997, Kingfisher Bay, Fraser Island, Queensland, Australia.

The organising committee welcomes your attendance at ANZMAG 97. This meeting incorporates the 10th Australian Magnetic Resonance Conference and follows the very successful joint meeting with ISMAR in Sydney in 1995 at which the Australian and New Zealand Society for Magnetic Resonance (ANZMAG) was inaugurated. The conference will cover all major areas of magnetic resonance including solution and solid state NMR and EPR.

The conference will be held at the Australian Tourism Award winning Kingfisher Bay Resort and Village on Fraser Island. World Heritage-listed Fraser Island is a unique natural wonder which lies at the southern end of the Great Barrier Reef. The island is the world's largest sand island and has 120km of sandy ocean beach, cliff faces of spectacular colour sands, lush tropical rainforests, freshwater streams, perched dune lakes and massive sand blows. The weather in December is superb with clear blue skies and warm temperatures.

The scientific programme will include:

- Biomolecular NMR
- Chemical Applications
- EPR
- Imaging/microscopy
- Instrument and technique development
- In vivo NMR
- Multinuclear NMR
- polymers/materials and Solid State NMR

The following speakers have accepted invitations to give plenary lectures at ANZMAG97: Ad Bax, National Institute of Health, USA, Paul Callaghan, Massey University, New Zealand, Stephen Fesik, Abbott Labs, USA, Les Field, University of Sydney, Australia, Hans Jakobsen, University of Aarhus, Denmark, Christina Redfield, Oxford University, UK, Claudia Schmidt, Universitat Freiburg, Germany, Arthur Schweiger, ETH, Switzerland, Peter Styles, Oxford University, UK, Gerhard Wider, ETH, Switzerland and Evan Williams, Varian Associates, USA.

The scientific program will be structured to allow ample opportunity for informal discussion and allow delegates to enjoy the delights of Fraser Island. For delegates bringing their family, the island offers a wide range of organised events which will run in parallel with the scientific program.

Further information and registration details can be obtained from the ANZMAG web site:

#### http://www.anzmag.com.au

Downloadable registration forms will available from this site in the near future. Requests for hardcopy registration brochures can be made by email to: anzmag@cmr.uq.edu.au. Or, contact the Secretary, Ian Brereton, Centre for Magnetic Resonance, The Univ. of Queensland, St. Lucia Qld., Australia 4072; 2: 61-7-3365-4100; FAX: 61-7-3365-3833.

Published at the Illinois EPR Research Center (IERC), Urbana, IL 61801, USA

# INTERNATIONAL SOCIETY for MAGNETIC RESONANCE in MEDICINE (ISMRM), 6th SCIENTIFIC MEETING and EXHIBITION, April 18-24, 1998, Sydney, Australia.

The 1998 Scientific Meeting of the International Society for Magnetic Resonance in Medicine will combine traditional and new elements of interest to both basic scientists and clinicians to provide a program to appeal to all attendees. Oral Scientific Sessions, Poster Sessions and Clinical Focus Sessions will be constructed from proffered abstracts. To guarantee the highest possible scientific quality and a fair selection of contributed presentations, each abstract will be reviewed by at least four peers. Plenary Lectures will be given on Monday through Friday. Of particular interest is the Lauterbur Lecture at the opening session. Plenary lectures will be given on topics with the most activity and progress today. Lectures will deal with clinical or physiological applications, methodological background, and functional/spectroscopic aspects. This should ensure that all groups of participants can benefit from this hopefully very dense transfer of scientific and clinical knowledge. Weekend Educational Courses will consist of lectures for beginners and advanced students. Traditionally, clinical magnetic resonance imaging is covered as well as magnetic resonance spectroscopy during these intense educational programs. Special Courses will be designed by the Educational and Scientific Program Committees in addition to the Plenary Lectures to cover specific upcoming and advanced questions.

Call for Papers. The Society invites submission of abstracts to be presented in oral and poster sessions. Abstracts must contain new, previously unpublished material. The deadline for receipt of abstracts in the ISMRM office is November 18, 1997. Abstracts accepted for presentation will be printed in the 24Proceedings for the meeting. Abstracts must be typed on official 1998 abstract forms. Detailed instructions are included with the forms. To receive abstract forms and instructions, please call, FAX, or write to ISMRM, 2118 Milvia St., Suite 201, Berkeley, CA 94704, USA; \$\mathbb{E}\$: 1-510-841-1899; FAX: 1-510-841-2340; E-mail: info@ismrm.org.

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

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

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

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

The Conference will include sessions devoted to the investigation of ESR and biologically relevant radiation effects in matter useful for therapy-level dosimetry as well as accident, retrospective and high-level dosimetry. Emphasis will be given to fundamentals, mechanisms and instrumentation. A wide variety of applications will be considered.

The primary intention of this Conference is to bring together experts from around the world in all these topics to promote communication on advances and to continue improvement of biodosimetry, applied dosimetry and material analysis particularly by ESR technology. It will be a pleasure to welcome our colleagues from abroad including the former Soviet Union countries and benefit from their expertise. The Conference will provide a forum for the exchange of ideas by the leaders in ESR and biological as well as biophysical dosimetry and their application in the important and expanding field of radiation dosimetry and metrology. The world-wide economic restrictions in research funding makes it meaningful to increase international and interdisciplinary co-operation.

Obninsk is a widely acknowledged scientific city with 14 big research centers functioning in various fields of fundamental and applied sciences. MRRC RAMS is one of them. It deals with medicine, particularly with radio oncology, radiobiology, radiation medicine and radiation epidemiology, and was concerned with the Chernobyl accident. The WHO Collaborating Center on Radiation Epidemiology and training has been established at MRRC RAMS. Obninsk is also known for the first nuclear power station in the world put in the operation in 1954. Obninsk is situated in the Kaluga Region at a distance of about 100 km south-west of Moscow. The population of the city is around 110.000. Tours to Obninsk research centers, Moscow, Kaluga and other nearest historical and cultural places will be offered to the conference participants and accompanying persons.

The Organizing Committee. President: Prof. A. Tsyb (Russian Academy of Medical Sciences); Co-President: Prof. L. Ilyin (Russian Academy of Medical Sciences); Vice-President and Programme Chairman: Dr. D. Regulla (GSF - Institut für Strahlenschutz); Scientific Secretaries: A. Romanyukha and V. Stepanenko; Local Organizers: A. Ivannikov, V. Skvortsov, Y. Skoropad (Russian Academy of Medical Sciences) and A. Panfilov and B. Lobach (Ministry of the Russian Federation for Atomic Energy, Moscow); Conference Logistics: U.A. Fill (GSF - Institut für Strahlenschutz); Editorial Board: M. Desoriers, S.S. Eaton, G.R. Eaton, W.L. McLaughlin and A. Skinner (USA); Scientific-Technical Exhibition: Y. Skoropad

Publication of the International EPR(ESR) Society

(Russian Academy of Medical Sciences) and U.A. Fill (GSF - Institut für Strahlenschutz).

*Preliminary topics* include:

- ESR Fundamentals
- Biodosimetry (molecular, cytogenetic and biophysical approaches to retrospective dosimetry)
- ESR Effects and Mechanisms (in biomaterials, organics and inorganics)
- ESR Retrospective Dosimetry (physical and technical bases and procedures
- Dose Intervention in Radiation Emergency
- Comparison of Individual Doses (from biological and physical methods)
- Biodosimetry and Health Effects
- Analysis of Uncertainty in Biodosimetry
- ESR Dosimetry in Medicine
- Reference, Transfer and QA Dosimetry
- ESR Spectroscopy in Radiation Chemistry
- Radation Processing, Food Irradiation and Identification
- Archeological and Geological Dating
- ESR Imaging and In Situ Dosimetry

Important Deadlines: Abstracts should be submitted by September 15, 1997. Early registration and payment of fees should be submitted by February 18, 1998 higher fees apply after that date. The latest date for submission of manuscripts for publication is June 26, 1998.

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

#### http://www.gsf.de/ESR/index.html

or by contacting the Programme Chairman and Vice President, Dr. D. Regulla, GSF-Forschungszentrum, Institut für Strahlenschutz, Postfach 11290, D-85764 Neuherberg, Germany; 2: 49-89-3187-2224; FAX: 49-89-3187-2517; Email: regulla@gsf.de OR the Conference President, Prof. A. Tsyb, or Co-President, Prof. L. Ilyin, Russian Academy of Medical Sciences, MRRC, 249020 Obninsk, Kaluga oblast, Russian Federation; 2: 7-095-956-1441; FAX: 7-095-956-1440; E-mail: mrrc@obninsk.ru.

# 29th AMPÈRE — 13th ISMAR INTERNATIONAL CONFERENCE on MAGNETIC RESONANCE & RELATED PHENOMENA, August 2-7, 1998,

#### Technische Universität Berlin, Berlin, Germany.

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

Scope of the Conference: The 29th AMPÈRE — 13th ISMAR Conference will cover a wide range of topics including fundamental aspects, new techniques, and applications of

Magnetic Resonance. It will be organized through plenary lectures, parallel Symposia, and Poster Sessions. Among others the following topics will be discussed:

- EPR, NMR, NQR, ENDOR, and μSR
- Developments in Liquid- and Solid-State NMR
- Spin Dynamics
- Non-equilibrium and Non-linear Phenomena
- Advances in Imaging and Microscopy
- Structure and Dynamics of Molecular Systems
- Molecular Material Science
- Proteins and Nucleic Acids Studies
- Membranes and Liquid Crystals
- In vivo NMR
- New Technologies and Experimental Methods

New Computational Methods and Software Satellite symposia are planned before the conference in Leipzig on the following topics:

- MR imaging (Organization: B. Blümich)
- NMR in surface and interphase science (Organization: J. Kärger, D. Michel)

Language: The official language of the Conference will be English.

Conference Site: The conference will be held at the Technical University of Berlin, located in the center of the city. It is served by subway (U-Bahn), S-Bahn, and bus lines. Berlin may be reached by train or by flights to Tegel, Tempelhof, or Schönefeld airports.

Accommodations and Social Program: Berlin provides hotels of different categories for the participants. A list of hotels of the requested category will be sent with the 2nd circular. Participants are expected to arrange booking directly with the hotel of their choice. Details of the social program will be given in the 2nd circular.

Registration: The registration fee is DM 500/400 (non members/members of the Groupement AMPÈRE and ISMAR), DM 150 for diploma and Ph.D. students (need letter of confirmation from the respective institute), DM 80 for accompanying persons.

*Publications*: A book of abstracts will be available to registrants upon arrival.

Second Circular: The second circular with the call for papers will be mailed in summer 1997. It will also be available on the web page:

#### http://ISMAR-CA98.tu-berlin.de

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

Organizing Committee: D. Ziessow, Chairman; W. Lubitz, Co-Chairman; F. Lendzian, Secretary; D. Haberland, Local Organization.

Program Committee: D. Ziessow (Berlin), W. Lubitz (Berlin), H. H. Limbach (Berlin), K. Möbius (Berlin), H. Oschkinat (Berlin), D. Stehlik (Berlin), B. Blümich (Aachen), K. P. Dinse (Darmstadt), C. Griesinger (Frankfurt/M), H. Günther (Siegen), A. Haase (Würzburg), U. Haeberlen (Heidelberg), H. Kessler (München), R. Kimmich (Ulm), G. Kothe (Freiburg), M. Mehring (Stuttgart), D. Michel (Leipzig), H. Rüterjans (Frankfurt/M), J.-M. Spaeth (Paderborn), H. W. Spiess (Mainz). In consultation with: M. Goldmann (France), President ISMAR; P. Servoz-Gavin (France), Secretary General ISMAR; B. Maraviglia (Italy), President Groupement AMP RE; R. Kind (Switzerland), Secretary General Bureau AMP RE. International Advisory Board: All members of the ISMAR Council, Committee AMPÈRE.

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

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

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

For further information on the XVIIIth ICMRBS, please contact Prof. M. Kainosho, Dept. Chemistry, Tokyo Metropolitan Univ. (TMU), Hachioji, Tokyo, Japan; 2: 81-426-77-2544; FAX: 81-426-77-2525; E-mail: kainosho@raphael.chem.metro-u.ac.jp.

## ADDITIONAL CONFERENCE UPDATES AVAILABLE on WORLDWIDE WEB.

The EPR Newsletter web page contains the latest information on conferences for which notices arrived after the publication deadline. The web address is:

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

### **POSITIONS AVAILABLE**

Postdoctorial fellowship available, NIEHS/NIH, Research Triangle Park, NC, USA. Biological ESR spectroscopist for investigations into protein-derived radicals, in vivo detection of radicals, and/or nitric oxide complexes. Less than five years postdoctorial experience with a Ph.D. in chemistry, biochemistry, pharmacology, or toxicology. Please

send curriculum vitae to Ronald P. Mason, Free Radical Metabolite Workgroup Leader, NIEHS/NIH, P.O. Box 12233, Research Triangle Park, NC, 27709, USA; **≈**: 1-919-541-3910; FAX: 1-919-541-5737.

Postdoctoral Position in Electron Spin Resonance. The Magnetic Field Laboratory National High Tallahassee/Florida invites applications for a postdoctoral research associate position. The starting date will be fall/winter 1997. The successful candidate will build, maintain, and operate a multi-user transient EPR spectrometer in high magnetic fields with ns and sub-ns time resolution. Applications of the new spectrometer will be in a wide range of areas, e.g., the study of fast transient paramagnetic species in photosynthesis, photochemistry, organic monolayers, muscle contraction, and non-linear optical materials. Candidates must possess a Ph.D. in physics, chemistry, or related disciplines. Experience in one or more of the following areas is preferred: 1. Transient ESR with high time-resolution (ns), 2. High-field ESR (W-band or higher), 3. Sub-ns to ps optical spectroscopy, 4. Quasi-optical techniques. We are looking for a self-motivated individual with broad scientific interests who enjoys working in a multi-disciplinary research laboratory. The position is available for 2 years, initially. Salary will depend on experience. Please, contact Dr. Louis-Claude Brunel, 2: 1-904-644-1647, FAX: 1-904-644-1366; E-mail: brunel@magnet.fsu.edu, for further information. Send CV and arrange for 3 letters of support to be sent to: Dr. Louis-Claude Brunel, National High Magnetic Field Laboratory, 1800 E. Paul Dirac Dr., Tallahassee, FL 32310,

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

Publication of the International EPR(ESR) Society

for 3 letters of reference to be sent directly to Professor Harold M. Swartz, Dartmouth Medical School, 7785 Remsen, Hanover, NH, 03755 USA; E-mail: harold.swartz@dartmouth.edu; FAX: 1-603-650-1130.

Research Assistant, City University of Hong Kong. There is a vacancy for a Research Assistant I/II to work on the project: "Spectroscopic studies of optoelectronic materials doped with transition metal and rare-earth ions." Start date: preferrably Sept 1997, duration: 10-12 months. Knowledge of EPR, crystal field theory & spin Hamiltonian theory of TM ions required. Inquiries and applications to: Prof. C. Rudowicz, City University of Hong Kong, Dept. of Physics & Mat. Sci., FAX: 852-2788-7830, E-mail: APCESLAW@CITYU.EDU.HK.

# EQUIPMENT & SUPPLIES EXCHANGE

#### WANTED: USED VARIAN SPECTROMETER

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

#### WANTED: BENCH-TOP EPR SPECTROMETER

We are looking for a bench-top EPR spectrometer, like an E-3. Does anyone have or know of an EPR which is collecting dust? We are short on cash, so price is important. Please contact Prof. Lew Cary, Dept. Chemistry, Univ. Nevada, Reno, NV 89506 USA; : 1-702-784-6019; E-mail: lcary@chem.unr.edu.

#### **WANTED: VARIAN E-4**

A replacement for our Varian E-4. Are you upgrading and would like to transfer your similar instrument under a low-budget arrangement? Contact Lance Crist, **3**: 1-202-687-1682; E-mail: crist@gusun.georgetown.edu.

#### **AVAILABLE: VARIAN MAGNET**

A Varian 9-inch EPR/NMR magnet is available. It includes fully functional Field dial Mark II power supply. The magnet is free, but you will pay the rigging and shipping charges. Contact Steve Greenbaum, Hunter College, Dept. Physics, 695 Park Ave., New York, NY, 10021, USA; 2: 1-212-772-4973; E-mail: steve.greenbaum@hunter.cuny.edu.

#### 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; \$\alpha/FAX: 1-773-728-6570.

#### WANTED: VARIAN MICROWAVE BRIDGE

One Varian X-band microwave bridge — Varian Model E-102. Contact: Lon B. Knight, Jr., Furman University, Department of Chemistry, Greenville, SC 29613, USA; 2: 1-864-294-3372; FAX: 1-864-294-3559; E-mail: knight\_lon/furman@furman.edu.

#### **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 COMPONENTS and MAINTENANCE

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

http://www.webspace.it/vpnmr

# **OFFERED: HELP in the DESIGN and CONSTRUCTION of EPR ELECTRONICS**

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 KHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a conversion kit to convert Varian field control units to voltage-controlled scan operation. A 6 digit 1 ppm frequency counter is available in X-, C-, S- or L-band or Megahertz versions. Complete microwave/RF bridges from 150 MHz to L-, S-, or C-band are available from designs previously built and tested at the Univ. Denver. Contact Richard W. Quine,  $\blacksquare$ : 1-303-871-2419; E-mail: rquine@du.edu.

#### FOR SALE: VARIAN SYSTEM

Resonance Instruments presently has available:

- 1) a E110 Q-band Bridge with cavity
- 2) replacement Klystrons for Varian EPR Bridges (at reduced prices)
- 3) Model V4533 VARIAN EPR TE011 mode, rotating cylindrical cavity
- 4) VARIAN general purpose cavity E231
- 5) VARIAN V4500-41A low/high power microwave bridge with new klystron—excellent condition
- X-band DEWAR probe outfitted with a tuner and with stainless steel waveguide

For more information on these units contact Clarence Arnow, President, Resonance Instruments. **2**: 1-847-583-1000; FAX: 1-847-583-1021; E-mail: mninco@wwa.com.

### **AVAILABLE: TWO IBM 9000 COMPUTERS**

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

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

### WANTED: USED X-BAND MICROWAVE BRIDGE

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

### **ANNOUNCEMENTS**

### MAILING LISTS FOR SCIENTIFIC MEETINGS

If you are planning a scientific conference, you may contact an officer of the IES or the IERC to obtain a list of the 1,400+ Society members for use in issuing invitations. If you would like mailing labels, Martha Moore, who provides secretarial support for the Society, can do this at cost -- approximately \$50.00 per 1,000 (includes cost of labels, postage and, if you wish, a disk copy of the list in ASCII format). Labels for the entire database (over 3,800 members and non-members) would cost about \$200.00. Ms. Moore can be reached by Email: IERC@uiuc.edu.

# MEMBERSHIP INFORMATION AVAILABLE ON THE WEB

A list of all members whom the IES records show as having paid dues in 1994, 1995, 1996, and/or 1997 is 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 update the list monthly; please allow time for recent payments to be placed on the list. 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 1997, a dues payment form is on this web site along with methods to pay dues, depending on where in the world you are located.

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