ELECTRON SPIN RESONANCE CENTERS NEWSLETTER

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ELECTRON SPIN RESONANCE CENTERS NEWSLETTER - Vol. 1, # 1 - July 31, 1987

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OUR FIRST ISSUE

This is the first issue of a new publication which is intended as a news bulletin and a medium for rapid and informal exchange of information among scientists in the ESR (i.e., EPR) community. This newsletter is edited and published by the staff of the Illinois ESR Research Center (IERC) and is a cooperative venture of the three national electron spin resonance centers which are sponsored by the Division of Research Resources of the National Institutes of Health:

1. The National Biomedical ESR Center at the Medical College of Wisconsin, Milwaukee, WI
2. The Illinois ESR Research Center at the University of Illinois at Urbana-Champaign, Urbana, IL, and
3. The Biotechnology Resource for Pulsed EPR Spectroscopy at the Albert Einstein College of Medicine, the Bronx, NY.

This issue contains a brief description of each of the Centers and explains how prospective users may contact them to discuss projects and arrange for use and assistance. In addition to news and more information from the Centers, future issues may include announcements of upcoming conferences and symposia, research notes, tips and brief descriptions of special techniques, positions-open and positions-wanted listings, or any other items that may be of interest to the ESR community. We invite your participation.

READER SURVEY

What should be included in these Newsletters? Is our mailing list accurate? We invite you to take a few moments to fill out the form at the end of this issue and return it to us.

HOW TO REACH US

To communicate concerning the ESR Centers Newsletter, write any of the IERC senior staff (Linn Belford, Bob Clarkson, Hal Swartz, Peter Debrunner, Mark Nilges, or Reef Morse) or Becky Gallivan, Editorial Assistant, at IERC, UIUC College of Medicine, 190 MSB, 506 S. Mathews, Urbana, IL 61801. Phone 217/244-1186 or use our BITNET computer link, BELFORD@UIUCSCS.

MEETINGS

Some meetings of interest within the next year are

Minisymposium: "Imaging and Related Studies by Electron Spin Resonance," Biophysics Society Meeting, Phoenix, Arizona. February 26 to March 3, 1988. Contact Prof. Harold M. Swartz, IERC, College of Medicine, University of Illinois, 190 MSB, 506 S. Mathews Ave., Urbana, IL, 61801 for details.

XIII Annual International Conference on Magnetic Resonance and Biological Systems, Madison, Wisconsin. August 14 to 19, 1988. Contact Prof. James S. Hyde, ESR Center, Medical College of Wisconsin, 8701 Watertown Plank Road, Milwaukee, WI, 53226 for details.

Eleventh International EPR Symposium at the 30th Annual Rocky Mountain Conference, Denver, CO. July 31 to August 4, 1988. Contact Prof. Gareth Eaton, Department of Chemistry, University of Denver, Denver, CO, 80208 or Prof. Sandra Eaton, Chemistry Department, University of Colorado at Denver, 1100 14th Street, Denver, CO, 80202 for details.

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MEETINGS -- continued

The 1988 Gordon Conference in Magnetic Resonance in Biology and Medicine will be held at the Tilton School, Tilton, NH. July 18 to 22, 1988. The conference is devoted to EPR and NMR studies of biological systems. Contact Prof. N. Dennis Chasteen, Department of Chemistry, University of New Hampshire, Durham, NH, 03824 for details.

NOMENCLATURE

EPR or ESR? Which shall it be, or does it matter? There are attempts to set international nomenclature standards. More about this in future issues!

USE OF THE CENTERS

All three national ESR Centers are generally open to all scientists, whether expert or inexperienced in ESR, whose research can be helped by application of ESR techniques. One purpose of the Centers is to provide experienced ESR spectroscopists with the opportunity to use specialized, sophisticated, and/or expensive facilities which they may not have in their own laboratories. However, the Centers (to varying extents) are also oriented towards helping scientists with little or no ESR expertise. One of the Centers' functions is to help investigators decide whether their problems can profit from ESR approaches.

DESCRIPTIONS OF THE CENTERS

The following pages contain brief descriptions of the three existing national ESR Research Resources. For more information about any one, or to inquire about use, contact one of the staff members designated in the description.

WHICH CENTER TO CONTACT

Over the past few years, electron spin resonance has grown in technical sophistication and variety. While the three existing ESR Centers have much in common, they also reflect that variety. They differ in several ways including subtle but substantial ones which may not be apparent from their published descriptions. If you are not certain which Center to contact, just call or direct your inquiry to whichever one seems most likely to be useful. You will be referred to the most appropriate Center for your purpose. All of the national Centers are in close communication, interact well, and collaborate in some problems. The staff members of each Center understand most of the strengths, capabilities, and emphases of the others.

NATIONAL BIOMEDICAL ELECTRON SPIN RESONANCE CENTER MILWAUKEE, WISCONSIN

The National Biomedical Electron Spin Resonance (ESR) Center was established in April 1976 at the **Medical College of Wisconsin** in Milwaukee, Wisconsin by a grant from the Division of Research Resources, Biotechnology Resources Branch of the National Institutes of Health.

Staff: Dr. **James S. Hyde** serves as Principal Investigator and Director of the Center. At present there are fifteen Ph.D. research scientists trained in ESR spectroscopy associated full time with the center. Four full- and two part-time degree-holding electrical engineers, and an electronics technician are employed. A machinist is employed halftime.

Equipment: There are six spectrometer systems at the center: ENDOR (Varian E-109 EPR spectrometer with E-1700 ENDOR accessory); ELDOR (Varian E-9 EPR spectrometer with E-800 frequency swept ELDOR accessory); multifrequency ESR (Varian E-9 with 500-1,000 MHz, 1-2 GHz, 2-4 GHz, 9 GHz, and 35 GHz bridges); time domain ESR (saturation recovery measurements of relaxation times); Varian E-4 ESR spectrometer system; IBM instruments ER 200D ESR spectrometer system.

Magnetometers and frequency counters are available for precise field and frequency measurements (including 35 GHz). Other pieces of equipment available include: on-line minicomputer for data acquisition and spectral simulation; vacuum line; photochemical facilities including Xe and Hg lamps and monochromator; high-power sonication; stopped-flow ESR apparatus; Perkin-Elmer 320 UV-VIS spectrophotometer; Sorvall RC5B super speed refrigerated centrifuge; Beckman Airfuge ultracentrifuge; Cahn balance (microgram sensitivity); and other normal chemical and biological laboratory equipment. Microwave test equipment including Hewlett-Packard sweep generator to 40 GHz (HP8690) and a spectrum-analyzer (HP8566). Extensive electronic test equipment. A new Janis variable temperature cryostat is currently being installed which will facilitate use of our microwave resonators down to liquid helium temperatures.

Capabilities: The Milwaukee ESR Center staff has broad experience in use of nitroxide radical spin labels to measure translational and rotational diffusion in biological systems, with particular emphasis on measurement of rotational correlation times in the range of 1 msec to 100 nsec and on the measurement of slow translational diffusion constants (10^{-6} to 10^{-9} cm^2/sec). These are characteristic values for components of biological membranes. Several spin probe methods have been developed and are available for measuring oxygen concentrations and diffusion in cells and other complex systems.

Identification, characterization and quantification of transient and stable free radicals are accomplished in various ways using several types of ESR equipment. Xenon and mercury lamps can be used to photochemically generate paramagnetic species in the ESR cavity. In addition, radicals can be produced in a mixing chamber and flowed into the ESR cavity within milliseconds. An X-band resonator and special mixing chamber requiring very small quantities of material is being completed. Personnel of the center have considerable experience in the techniques of spin trapping, spin stabilization, determination of quantum yield and action spectra.

It is often possible to identify paramagnetic metal ions and determine the symmetry of the crystal field, the charge, and the ligation. Cu is being used as an extrinsic probe of the structure of metal-binding sites, primarily using the 2-4 GHz bridge. The 2-4 GHz microwave frequency range has been found to give maximum resolution of the nitrogen superhyperfine structure of square-planar copper complexes. With this improved resolution and a sophisticated computer simulation it has been possible to determine the number nitrogen atoms bound to copper. Study of relaxation processes by means of which paramagnetic centers are maintained in thermal equilibrium with their environment is possible, using the recently developed pulse ESR spectrometer.

Areas of current research include: Physical studies of nitroxide radical spin labels; measurement of spin-label T_1's; diffusion processes in synthetic and biological membranes; measurement of oxygen concentrations in synthetic membranes and of oxygen uptake in cellular systems; spin-label studies of fibronectin; physical studies of melanin; clinical and diagnostic studies of melanin-containing tissues; ESR characterization of immobilized free radicals; phototoxicity in pigmented tissues; oxidation mechanisms and toxicity of catecholamines; spin-trapping and spin-stabilization of oxygen-centered free radicals; copper ligation and charge in copper proteins and copper-containing chemotherapeutic and radiosensitizing drugs; and characterization of higher order effects occurring in transition metal spectra at low microwave frequencies.

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

A limited number of young scientists (5 to 10) are invited each year to spend 2 weeks at the center to obtain experimental knowledge of advanced or specialized ESR techniques.

Whom to contact: The persons to contact about using the center or obtaining more information are

Christopher C. Felix, Ph.D.
[Tel. (414) 257-8760]

or

James S. Hyde Ph.D.
[Tel. (414) 257-8570]

Mailing address:

ESR Center
Medical College of Wisconsin
8701 Watertown Plank Rd.
Milwaukee, WI 53226.

BIOTECHNOLOGY RESOURCE IN PULSED EPR SPECTROSCOPY BRONX, NEW YORK

The Biotechnology Resource in Pulsed EPR Spectroscopy, located at **Albert Einstein College of Medicine** in the Bronx, NY, was established in September, 1985 under a grant from the Division of Research Resources, NIH. The Principal Investigator is **Jack Peisach**, Ph.D.

I. Services Available

Instruments: The Resource includes the following EPR instruments: a pulsed EPR spectrometer for performing Electron Spin Echo (ESE) experiments over a microwave frequency range of 8-18 GHz with microwave pulse power up to 1 kW and minimum pulse widths of 10 nsec; a Varian E-112 cw-EPR spectrometer operating at X-band; and a Bruker ER 200D X-band cw EPR spectrometer with EN-810 ENDOR accessory.

Special Features: Special features of the pulsed EPR instrument are: cryogenic measurements to $1.3^{O}K$; pulse programmer time resolution of 1 ns; equipment for performing linear electric field effect (LEFE) measurements; stripline and folded stripline cavities to accommodate samples in 4 mm O.D. quartz tubes; microprocessor control; and LSI 11/73 and Microvax II work stations for data analysis including fast Fourier transformation and simulation of ESE envelope modulation data. Among the accessories available for use with both pulsed and cw EPR instruments are an NMR gaussmeter, microwave frequency counter, and cryogenic equipment. The facility is housed in a standard biochemistry laboratory that contains extensive equipment for sample preparation and characterization including a Perkin-Elmer model 5000 AA Spectrometer, an Aviv Model 14DS UV-Vis-IR spectrophotometer, a Tracor Northern TN-6050 diode array UV-Vis spectrophotometer, centrifuges, and a cold room. Also available are microwave and electronic test equipment including an HP8690 microwave sweep oscillator (0.1-110 MHz, 4-40 GHz).

Service Personnel: Resource personnel maintain and operate spectrometers and computer equipment. Training of users in spectrometer operation and analysis of ESE data is available upon request. Research is either of a collaborative or service oriented nature.

User Laboratory Space: provided.

II. Research Emphasis or Application

Data Achievable with Resource's Methodologies: This Resource provides the investigator with a means for measuring hyperfine and superhyperfine interactions between magnetic nuclei and paramagnetic centers through the use of ESE envelope modulation techniques and cw-ENDOR. Because these hyperfine splittings are often not detected by cw EPR methods, the techniques are particularly well suited for the study of paramagnetic biomolecules. For both ESE and ENDOR, one can relate the observed spectroscopic splittings to the identity of the nuclei giving rise to the effect and can parameterize the magnetic coupling between those nuclei and the paramagnet. These coupling parameters provide a means for characterizing ligand bonding and, in some cases, the distance of a particular ligand nucleus from the paramagnetic center. ESE envelope modulation studies provide additional information concerning ligand group identity and the number of such ligands bound. Therefore, these studies can yield much information concerning the structure about a paramagnetic center and how that structure is altered by chemical or biochemical processes. LEFE measurements using the ESE technique can provide information concerning crystal field symmetry for paramagnetic metalloproteins, metal complexes and transition metal model compounds.

Current Research: We are currently performing ESE envelope modulation studies of metalloproteins, metal-drug complexes, transition metal model complexes and radical species of biological importance. The questions being addressed concern the ligation structure about paramagnetic metal centers in these systems and how those structures change when various substrates or inhibitors are added. Model compound studies have focused on providing the framework for interpreting protein data and understanding ESE envelope modulation data from first principles. The development of computer software for analysis of these data and the development of pulsed EPR instrumentation to enhance sensitivity for the study of biological materials are also primary functions of the Resource.

New Capability: New capabilities being added to the Resource include extension of the microwave frequency range of the ESE spectrometer to C-band (4-8 GHz) and development of spin-echo ENDOR for use by the biological community.

Recent Publications:

1. McCracken, J., Peisach, J. and Dooley, D.M. (1987). Cu(II) coordination chemistry of amine oxidases: Pulsed EPR studies of histidine imidazole, water and exogenous ligand coordination. J. Am. Chem. Soc., in press.

2. Dooley, D.M., McGuirl, M.A., Peisach, J. and McCracken, J. (1987). The generation of an organic free radical in substrate-reduced pig kidney diamine oxidase-cyanide. FEBS Lett., in press.

3. Magliozzo, R.S., McCracken, J. and Peisach, J. (1987). Electron-nuclear coupling in nitrosyl heme proteins and in nitrosyl ferrous and oxy cobaltous tetraphenylporphyrine complexes. Biochemistry, in press.

4. Mondovi, B., Morpurgo, L., Agostinelli, E., Befani, O., McCracken, J. and Peisach, J. (1987). A comparison of the local environment of Cu(II) holo and half Cu-depleted bovine serum amine oxidases. Eur. J. Biochemistry, in press.

5. McCracken, J., Pember, S., Benkovic, S.J., Villafranca, J.J., Miller, R.J. and Peisach, J. (1987) Electron spin echo studies of the copper binding site in phenylalanine hydroxylase from Chromobacterium violaceum. J. Am.Chem. Soc., submitted.

Whom to contact: The persons to contact about using the resource or obtaining more information are

John McCracken, Ph.D.
[Tel. (212) 430-2175]
or
Jack Peisach, Ph.D.
[(212) 430-2175]

Mailing address:

Albert Einstein College of Medicine
Department of Molecular Pharmacology
1300 Morris Park Avenue
Bronx, NY 10461

UUCP Network Address: **peisach@aecom**

ILLINOIS ESR RESEARCH CENTER
URBANA-CHAMPAIGN, ILLINOIS

The Illinois ESR Research Center (**IERC**), located at the **University of Illinois** at Urbana-Champaign, was established in September, 1985, under a grant from the Division of Research Resources, NIH; the Principal Investigators are Profs. **Harold M. Swartz**, M.D., Ph.D. (Depts. of Biophysics and Medicine), **R. Linn Belford**, Ph.D. (Dept. of Chemistry), **Robert B. Clarkson**, Ph.D., Dept. of Medicine), and **Peter G. Debrunner**, Ph.D. (Dept. of Physics).

Staff: Profs. Swartz and Belford serve as co-Directors and Prof. Clarkson as Associate Director of the IERC. Other personnel include Mark J. Nilges, Ph.D. and Philip D. Morse II, Ph.D., who manage the laboratory, assist users, and conduct some of the core research and development. Ms. Rebecca J. Gallivan serves as the Administrative Assistant. In addition, there are over thirty senior scientists, postdoctorals, and graduate students associated with the IERC.

Facilities: <u>Instrumentation.</u> ESR spectrometer systems include a Varian E-109 X-band system; Varian E-112 X-band system; Varian E-15 Q-band system; Bruker ER-200D spectrometer; Bruker ER-200 spectrometer; locally-constructed X-band spectrometer; Varian E-1700 ENDOR accessory (50 kHz to 120 MHz) with upgraded radiofrequency sweep system; Bruker ENDOR accessory; Oxford liquid helium cryostat for use on Bruker ESR and ENDOR systems; Air Products liquid helium cryostat for use on both Varian and Bruker spectrometers; L-band (ca. 1.3 GHz) bridge with provisions for use with a axial air-core magnet (0 to 0.1T) to allow experiments with parallel static and microwave oscillating magnetic fields; ESR imaging accessories for 1.5 and 9 GHz; Varian and Bruker variable temperature accessories; tracking gaussmeters (two Bruker, one Varian); frequency counters (rf to 100 GHz); two field-frequency locks; several cavities (single, dual, dual mode, optically accessible, loop-gap, confocal, etc.).

Auxiliary instrumentation includes apparatus for flash photolysis or continuous UV irradiation of samples and visible-UV spectrophotometry. The ESR, including ENDOR, instruments have digital microcomputer-driven control and data acquisition capability.

Instruments under construction include a High Frequency ESR operating at W band (95 GHz) with sweeping superconducting magnet (experimental operation anticipated in 1988); S-band (2-4 GHz) CW/pulsed ESR spectrometer (trial operation anticipated 9/87 in CW; early 1988 in ESE mode); 1-2 GHz <u>in vivo</u> ESR spectrometer (experimental operation planned for early 1988).

<u>Computation</u>: Computer facilities in the IERC laboratories include several IBM-PC XT, AT, and compatible microcomputers, Bruker Aspect, IBM 9000 systems, PDP-11, and access by terminals in the laboratories to DEC VAX 11/780 with FPS array processor, Cray supercomputer, CDC Cyber, and IBM mainframe computers and a variety of peripherals. Capabilities exist for theoretical simulation of ESR, ENDOR, and ESE spectra from single crystals, powders, and liquids, with the ability to choose spectral parameters for the best fit between theoretical and experimental data. Data transfer between IERC and other laboratories <u>via</u> BITNET is routine (see below).

<u>Laboratories, Shops, and Auxiliary Services:</u> IERC laboratories contain the usual range of appointments for chemical, biochemical, and biomedical work, including tissue culture facility,

hoods, vacuum lines, preparation stations, and some shop facilities. The IERC has access to a wide variety of campus services including glassblowing, printed circuit fabrication, NMR and mass spectrometry, machining, electronics design and construction, and chemical microanalysis. Liquid nitrogen and liquid helium are supplied locally.

Service Personnel and Policies for Use: Resource personnel are available for consultation and collaborative research on various aspects of biological, biochemical, or physical-chemical application of ESR spectroscopy available at the Center. Users may stay for short- or long-term studies. After instrument training, they run their own experiments, usually in collaboration with Center personnel. Spectroscopic service on samples submitted for investigation is provided on an occasional basis. User laboratory space is available as needed for biological, chemical, or biochemical studies. Since this campus has many potential users of this Center, IERC policy is to give off-campus users first priority to prevent local preemption of instrument usage.

Research Emphasis: Experiments possible with IERC facilities: Multifrequency ESR provides an experimental route to study the interactions present in paramagnetic materials. The materials may be naturally paramagnetic — radicals or metal ions — or induced to be paramagnetic by introduction of spin labels (e.g., nitroxides or transition metal ions) or radiation. The ability to choose frequencies over a wide range — two orders of magnitude — allows selection for optimum resolution of particular features and tuning of the relative contributions of Zeeman and zero-field terms characterizing the specimen. Investigating short-range order in powders, glasses, interfaces, and frozen solutions with multifrequency ESR, ESE, and ENDOR is emphasized here. High sensitivity for small samples, resolution of overlapping spectral features, and access to transitions with large zero-field splittings are aims of higher frequencies (existing Q-band system and W-band system being constructed). Techniques are available to monitor reaction kinetics and to study motional effects and spin relaxation. Biomedical and materials applications are emphasized.

Current activities include: Applications of ESR to viable biological systems; characterization of contrast agents for NMR imaging; measurement of oxygen and redox metabolism in biological systems; ESR imaging; development of high frequency ESR; studies of local order in powders and frozen solutions using ENDOR and ESE spectroscopies; development of 2 - 4 GHz ESE spectrometer; research in ESR and ENDOR theory, including simulation methods.

Whom to contact: The persons to contact about using the IERC facilities or obtaining more information are

Mark J. Nilges, Ph.D.
[Tel. (217) 333-3969]
or
Philip D. Morse, II, Ph.D.
[Tel. (217) 333-3969]
or
Profs. Clarkson, Belford, or Swartz
[c/o Ms. Gallivan, (217)-244-1186]

Mailing address:
Illinois ESR Research Center
College of Medicine
University of Illinois
190 Medical Sciences Building
506 S. Mathews Street
Urbana, IL 61801

Electronic mail and file transfer:

BITNET address: **BELFORD@UIUCSCS.** Messages take a few minutes to a day, while long files may take a day or so.

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IN THIS ISSUE

HOW TO REACH US

To communicate concerning the ESR Centers Newsletter, write any of the IERC senior staff (Linn Belford, Bob Clarkson, Hal Swartz, Peter Debrunner, or Mark Nilges) or Becky Gallivan, Editorial Assistant, at IERC, UIUC College of Medicine, 190 MSB, 506 S. Mathews, Urbana, IL 61801. Use our BITNET computer link, BELFORD@UIUCSCS, or phone 217/244-1186. We welcome news items, notices of events, and appropriate articles for possible publication in this Newsletter. Our choices of material to be published will be strongly influenced by the opinions many of you expressed in response to our first issue.

MEETINGS

Among the forthcoming meetings of interest to EPR scientists are the following:

Twenty-Second International Meeting of the United Kingdom E.S.R. Group, University of Sheffield, Sheffield, England. April 10-14, 1989. The theme will be ESR of metals in inorganic and bioinorganic systems. For details, contact Dr. J. Barrie Raynor, Dept. of Chemistry, The University, Leicester LE1 7RH, England, U.K.

ESR Workshop, National Biomedical ESR Center, Milwaukee, May 12-13, 1989. For more details, see *News from the Centers* on page 2.

Third Chianti Workshop. Magnetic Resonance Workshop on Relaxation. To be held in Italy, May 28 to June 2, 1989. For more information, contact Jim Emsley, Scientific Co-Chairman, Dept. of Chemistry, The University, Southampton SO9 5NH, England, U.K.

Twelfth International EPR Symposium at the 31st Annual Rocky Mountain Conference, Denver, CO. July 30 to August 3, 1989. For details, contact Prof. Gareth Eaton, Dept. of Chemistry, University of Denver, Denver, CO, 80208 or Prof. Sandra Eaton, Chemistry Dept., University of Colorado at Denver, 1200 Larimer Street, Denver, CO, 80204, USA.

International Workshop on in-vivo ESR and ESR Imaging, L'Aquile, Italy. September 13-15, 1989. For details, contact Prof. P. L. Indovina, Laboratorio delle Radiazioni, Istituto Superiore di Sanita, Viale Regina Elena 299, 00161 Roma, Italy.

International Conference on Nitroxide Radicals, Novosibirsk Akademgorodok, USSR. September 18-22, 1989. Sponsored by IUPAC and organized by the Academy of Sciences of the USSR. For details, contact Dr. V. V. Martin, Institute of Organic Chemistry, Siberian Division of the Academy of Sciences of the USSR, Novosibirsk-630090, USSR.

SHOULD AN EPR (ESR) SOCIETY BE ESTABLISHED?

by Harold M. Swartz, IERC

It has been suggested that the ESR community would benefit by establishing its own formal society. For example, it might be beneficial to have a mechanism whereby credible input could be given to organizations such as research funding agencies (*e.g.*, NIH, NSF, DOE in the USA) and commercial manufacturers on issues and needs related to ESR techniques and instruments.

A major reason for proposing an EPR/ESR society is that, although most of us belong to several societies, those that focus on magnetic resonance tend to be dominated by NMR. I sit on the Board of Directors and Steering Committee of two of these organizations, where my most prominent input usually is to remind my colleagues that, in their deliberations and/or written materials, they have taken NMR to encompass the entire society!

The other functions usually associated with a scientific society might be useful to the ESR community. For example, such a society should facilitate the organization and staging of special workshops, meetings, and the like. It also would provide a systematic mechanism for listing of positions and events and perhaps for seeking support for students and members to attend ESR meetings.

If such a society were to be organized, I believe that it should take advantage of existing structures and avoid unnecessary duplication. The ESR Centers Newsletter could be expanded in scope and frequency of publication to become the official newsletter for such a society. Rather than adding to our busy schedules a new regular meeting for the society, we might use the annual International EPR Symposium, organized by the Eatons, as our regular and official annual meeting. At this time, a new journal does not seem necessary.

You are invited to provide input on this proposal by returning the response sheet appended to this Newsletter or by BITNET. (See "How to Reach Us" on p. 1)

NEWS FROM THE CENTERS

From the ESR Center in Milwaukee:

The National Biomedical ESR Center at the Medical College of Wisconsin-Milwaukee has just moved into a new building. The new address is **National Biomedical ESR Center, Medical College of Wisconsin, MACC Fund Research Center Building, 8701 Watertown Plank Road, Milwaukee, Wisconsin 53226**. The new general telephone number is **414/266-4000**. An inauguration ESR Workshop will be held May 12-13, 1989. The first day will be devoted to LOOP GAP RESONATORS. On the second day, three parallel groups will be formed to discuss spin labels, free radicals, and organometallics. To receive more information about the workshop, please contact Dr. Christopher C. Felix at the above address.

A paper entitled "Murine L-Band ESR Loop-Gap Resonator," by W. Froncisz, T. Oles, and James S. Hyde, is in press in the Journal of Magnetic Resonance. Mechanical drawings of this resonator are available without charge to interested persons from James S. Hyde, Ph.D., Professor of Radiology and Biochemistry, Director, National Biomedical ESR Center; address above.

From the IERC in Urbana:

The S-band pulsed (Electron Spin Echo) spectrometer is in operation. While it is still in the trial stage and is being modified constantly, it is now possible to discuss possible collaborative experiments with outside users. Contact Bob Clarkson or Linn Belford if you are interested.

The IERC is collaborating with the National Institute for Standards and Technology (NIST, formerly the National Bureau of Standards) to develop new standard samples for EPR calibration. Although the project is still in its early stages, we expect it to result in the production and sale by NIST of certified EPR standard samples. Please use the attached Response Sheet to tell us what kind of standard you would find most useful.

Dr. Phillip D. ("Reef") Morse has resigned his position as Laboratory Manager at IERC to become Associate Professor of Chemistry and Biology at Illinois State University at Normal, Illinois, 61761, and has formed a company to develop and market laboratory software for EPR and other spectroscopic applications. However, since Reef will continue to be associated with IERC, inquiries about his EPR data-acquisition and manipulation program EW may still be sent to him at this address.

Prof. R. Linn Belford has received the 1988 John R. Kuebler Award, the highest award bestowed by Alpha Chi Sigma, the national chemistry professional fraternity. A national award is given every two years for outstanding contributions to the fraternity and to the profession. The award ceremony was held in July at the University of California in Berkeley.

THE FUTURE OF EPR INSTRUMENTATION

by Gareth R. Eaton* & Sandra S.Eaton**

* Department of Chemistry. University of Denver, Denver, CO, USA 80208
** Department of Chemistry, University of Colorado-Denver, Denver, CO, USA 80204

INTRODUCTION.— Predictions are difficult, especially about the future. However, to predict what commercial spectrometers will be like ten years from now, one should take a close look at what is being done today in some of the leading research laboratories. On August 7, 1987, over 65 scientists from universities, national laboratories, and industry in 14 countries gathered in Denver to examine the state of the art in EPR instrumentation and techniques and to design the EPR spectrometer of the 1990's.

The 10th International EPR Symposium, which immediately preceded the Workshop, illustrated the state of the art in many aspects of EPR. The morning session of the workshop provided a concise and comprehensive survey of current capabilities in spectrometer design, experimental technique, and software. The truly exciting possibilities revealed in these presentations fueled some "blue-sky" designing of the EPR spectrometer(s) of the 1990's. The following is a brief summary of the consensus of the Workshop. A more detailed report has been published in the Bulletin of Magnetic Resonance[1].

SUMMARY DESIGN CRITERIA.— Following vigorous discussion of the state of the art, and speculations about future needs and capabilities, it is clear that one spectrometer will not satisfy all needs. There is a clear and understandable difference of opinion between those who advocate the development of the ultimate sensitivity CW X-band spectrometer and those who advocate development of broadband and pulsed spectrometers.

A. Frequency Range.— It was agreed that one EPR spectrometer of the 1990's should be a 3-15 GHz broad-band system. This should become the new standard, replacing the ca. 9-9.6 GHz spectrometer as the routine spectrometer of the future. The sensitivity and resolution goal of this design should be what one can achieve today with a narrow-band X-band spectrometer. It will use a solid-state oscillator instead of a klystron, and the bridge will include both CW and saturation recovery capability. This instrument will require development of certain microwave components. A crucial part of the construction of this spectrometer will be to communicate to microwave engineers the need for, and challenge to make, the necessary broad-banded items.

Because of the central utility of X-band, there should also be a narrow-band instrument optimized for sensitivity and signal-to-noise ratio at ca. 9-9.6 GHz. The very best that one can achieve in this frequency range is critical to important scientific questions.

Q-band remains a good choice for a higher frequency. This, and some very low frequency, say in the 1-2 GHz range, should be available as accessories to the other spectrometers. Very low and very high frequencies relative to the 3-15 GHz standard range will be available primarily in a few research laboratories and NIH-funded research resource centers.

B. Pulse vs. CW.— Will CW or pulsed EPR be the standard in 10 years? How many CW and Pulse capabilities should be in the same box? The best guess is that the standard spectrometer should continue to be CW. However, it is so easy to put saturation recovery into the CW bridge, and saturation recovery is so important, that the standard research bridge should include it.

The complexities of pulsed EPR require quite a different bridge than that in the CW spectrometers, although CW capability can be included in the pulsed EPR bridge. Pulsed (spin echo) EPR and FT EPR will merge, and a standard pulsed bridge should include both capabilities. Both of these will be powerful tools for spectral studies of narrow-line spectra, such as nitroxyls, and for relaxation time, ESEEM, and dynamic studies of broader spectra.

C. Magnets.— For many years one expects to continue to use large electromagnets at least for the research spectrometers. Some limited application spectrometers might use permanent magnets plus sweep coils. In the "blue sky" future, high temperature superconducting materials may change the type of magnets used in EPR, but no such application is expected in the next ten years. Note that the use of a solenoid brings with it new points of view about access to the sample area and direction of B_0 relative to the microwave path.

D. Computers.— The spectrometer system should have computer control only. Very powerful computers will be plug-in modules, continuing the evolution from vacuum tubes through transistors, then integrated circuits to microprocessors, as the units of which we construct spectrometers. There is no sense in putting in all of the extra circuitry needed to permit manual control of each function.

There will be two computers, one intimately tied to the hardware of the spectrometer for data acquisition, and a second, independent of the spectrometer configuration, to be a workstation for data analysis and simulation. The first computer should be specialized to the spectrometer, with interrupt structure, etc., designed as a component of the spectrometer, and using a standard bus structure so that, *e.g.*, memory cards from third parties are readily available. It should have the computational power needed to run the spectrometer and provide temporary storage and preliminary display of the spectrum.

The attached workstation computer will have the major computational power for data manipulation and display, and most of the data storage. This computer would be selected largely for the software it could run, its speed of computation, and the quality of its graphical display. These workstation computers could use a wide range of software and could be the cheapest, fastest computer available at any time, replaceable in the system without affecting the hardware or software of the EPR spectrometer. Standard computer buses will be used, and standard communications links will connect the two computers to each other and to other computer networks. Ease of file transfer between the computers in both directions is essential. Ethernet may be the best current choice for file transfer.

OVERVIEW.— How good are these predictions? Over a ten-year period the overall proportion of research in, *e.g.*, metal complexes or diffusion studies will probably change slowly enough so that the estimates about which spectrometer capabilities will be needed are probably reasonable. However, scientists work with the tools they have, and usually push them to the limit of the performance they were designed for. Marketing of spectrometers is demand-driven, but research is resource-driven. We can only hope that the aggregate market will permit manufacturers of EPR spectrometers to provide some leadership *via* marketing of spectrometers with capabilities that many researchers don't yet know that they need.

FOLLOW-UP.— Because of concern that these discussions might have no impact beyond stimulating those who happened to be in the room, it was agreed to set up an *Ad Hoc* Committee on the Future of EPR Instrumentation. The members will be directors from the three NIH-supported national EPR Centers, and three other scientists:

Dr. James S. Hyde, National Biomedical ESR Center, Medical College of Wisconsin, MACC Fund Research Center Building 8701 Watertown Plank Road, Milwaukee, Wisconsin 53226.

Dr. Jack Peisach, Biotechnology Resource in Pulsed EPR Spectroscopy, Albert Einstein College of Medicine, Department of Molecular Pharmacology, 1300 Morris Park Avenue, Bronx, NY 10461.

Dr. Harold M. Swartz, Illinois ESR Research Center, College of Medicine, University of Illinois, 190 Medical Sciences Building, 506 S. Mathews Street, Urbana, IL 61801.

Dr. Jack H. Freed, Baker Laboratory of Chemistry, Cornell University, Ithaca, NY 14850.

Dr. Michael K. Bowman, Argonne National Laboratory, Chemistry Division, 9700 S. Cass Avenue, Argonne, IL 60439.

Dr. Gareth R. Eaton, Department of Chemistry, University of Denver, Denver, CO 80208 (coordinator of committee).

This committee will:

a. provide a communications focus for the EPR community,
b. periodically update the results of the Workshop,
c. keep abreast of funding trends,
d. report to the EPR community via the ESR Centers Newsletter,
e. offer advice to anyone who will listen (*e.g.*, NIH, NSF, corporations), and
f. meet formally at the annual International EPR Symposium in Denver and at other scientific meetings as the opportunity presents itself.

Comments on this analysis of the future of EPR instrumentation should be directed to a member of this committee for further discussion.

ACKNOWLEDGMENT.— The Workshop on the Future of EPR Instrumentation was organized with assistance from Dr. Caroline Halloway and was sponsored by the NIH Division of Research Resources.

[1] FOOTNOTE.— Volumes 10, No. 1/2 of the Bulletin of Magnetic Resonance is a special issue devoted to papers from the 10th International EPR Symposium and the Workshop on the Future of EPR Instrumentation. To order copies, contact Professor David Gorenstein, Editor, Bulletin of Magnetic Resonance, Department of Chemistry, Purdue University, West Lafayette, Indiana 47907, USA.

ELECTRON SPIN RESONANCE CENTERS NEWSLETTER

Published by the Illinois ESR Research Center (IERC), Urbana, IL 61801
Volume 1, #3, July, 1989

This Newsletter is a joint publication of the three national Centers for ESR spectroscopy. These Centers are sponsored by the Division of Research Resources of the U.S. National Institutes of Health:

National Biomedical ESR Center, Prof. James S. Hyde, Director. Medical College of Wisconsin, MACC Fund Research Center Building, 8701 Watertown Plank Road, Milwaukee, Wisconsin 53226, USA. Phone: 414/266-4000. E-Mail: felixc@medcolwi.BITNET.

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

Illinois ESR Research Center (IERC), Profs. Harold M. Swartz and R. Linn Belford, Directors; Prof. Robert B. Clarkson, Associate Director; Prof. Peter G. Debrunner, co-Principal Investigator. University of Illinois at Urbana-Champaign, 190 Medical Sciences Building, 506 S. Mathews, Urbana, Illinois, 61801, USA. Telephone: 217/244-1186. E-mail: belford@uiucscs.BITNET. FAX: 217-244-8068.

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

IN THIS ISSUE

HOW TO REACH US

To communicate concerning the ESR Centers Newsletter, write any of the IERC senior staff (Linn Belford, Bob Clarkson, Hal Swartz, Peter Debrunner, Mark Nilges, or Peter Gast) or Becky Gallivan, Editorial Assistant, at IERC, UIUC at Urbana, IL. We welcome news items, announcements, notices of events, and appropriate articles pertinent to ESR for possible publication in this Newsletter. Your comments are invited.

NOTICES OF MEETINGS

Twelfth International EPR Symposium at the 31st Annual Rocky Mountain Conference, Denver, CO. July 30 to August 3, 1989. For details, contact Prof. Gareth Eaton, Dept. of Chemistry, University of Denver, Denver, CO, 80208 or Prof. Sandra Eaton, Chemistry Dept., University of Colorado at Denver, 1100 14th Street, Denver, CO, 80202, USA.

Eighth Annual Scientific Meeting and Exhibition of The Society of Magnetic Resonance in Medicine, Rai Congrescentrum, Amsterdam, The Netherlands. August 12-19, 1989. For more information, contact The Society Business Office, 1918 University Avenue, Suite 3C, Berkeley, CA, 94704, USA.

Imaging in Medicine and Biology: Current Issues and Prospects, Philadelphia, PA, September 6-8, 1989. Sponsored by the Louis and Bessie Stein Foundation and Drexel University. For details, contact Dr. Dov Jaron, Biomedical Engineering and Science Institute, Drexel Univ., Philadelphia, PA 19104, USA.

International Workshop on in-vivo ESR and ESR Imaging, L'Aquile, Italy. September 13-15, 1989. For details, contact Prof. P. L. Indovina, Laboratorio delle Radiazioni, Istituto Superiore di Sanita, Viale Regina Elena 299, 00161 Roma, Italy.

International Conference on Nitroxide Radicals, Novosibirsk Akademgorodok, USSR. September 18-22, 1989. Sponsored by IUPAC and organized by the Academy of Sciences of the USSR. For details, contact Dr. V. V. Martin, Institute of Organic Chemistry, Siberian Division of the Academy of Sciences of the USSR, Novosibirsk-630090, USSR.

Twenty-first Annual Southeastern Magnetic Resonance Conference, Memphis, Tennessee, October 6-7, 1989. For details, contact Dr. Richard Petersen, Department of Chemistry, Memphis State University, Memphis, TN 38152, USA. Phone 901-678-4416.

Winter Meeting of the Society for Free Radical Research, "Free Radicals and Cancer," Eberhard-Karls-Universität Tubingen, Medizinische Klinik und Poliklinik, Federal Republic of Germany, December 8-9, 1989. Four scientific sessions and two workshops. For more information, contact Dr. M. R. Clemens, Medizinische Klinik, Otfried-Muller-Strasse 10, D-7400 Tubingen, F.R.G.

ELECTRON SPIN RESONANCE CENTERS NEWSLETTER
Published by the Illinois ESR Research Center (IERC), Urbana, IL 61801
Volume 1, #3, July, 1989

Twenty-Third International Meeting of the ESR Group of the Royal Society of Chemistry, Royal Holloway and Bedford New College, Egham, Surrey, England. March 26-30, 1990. The theme will be radicals in organic and bio-organic systems. For details, contact Dr. C. C. Rowlands, Secretary, Committee of the ESR Group. School of Chemistry, Univ. of Wales, PO Box 912, Cardiff CF1 3TB, U.K.

Thirteenth International EPR Symposium at the 32d Annual Rocky Mountain Conference, Denver, CO. July 29 to August 2, 1990. For details, contact Prof. Gareth Eaton, Dept. of Chemistry, University of Denver, Denver, CO, 80208 or Prof. Sandra Eaton, Chemistry Dept., University of Colorado at Denver, 1200 Larimer Street, Denver, CO, 80204, USA.

NEWS FROM THE CENTERS

From the National Biomedical ESR Center in Milwaukee: *Loop Gap Resonator Workshop:* As announced previously in the ESR Center Newsletter, a two-day workshop on loop gap resonators was held in Milwaukee on May 12 and 13, 1989. Attendance was about 85 persons from outside the city, with 25 more local attendees. The program and scientific handouts are available to interested persons. Included in the handouts is a reproduced collection of 19 papers on loop gap resonators. Write to Dr. Christopher C. Felix.

National Biomedical ESR Center Advisory Committee: Prof. Betty J. Gaffney has resigned as a member of the Advisory Committee and Prof. Gareth R. Eaton has accepted appointment as her replacement. The extramural members of the committee are D. C. Borg, H. M. Swartz, B. M. Hoffman, G. R. Eaton, and W. L. Hubbell. Prof. Helmut Beinert serves as chairman. These persons stand ready to not only advise the Center Director (Dr. Hyde) but also to represent and serve the community of users of the National Biomedical ESR Center.

Update on Multifrequency Saturation Recovery at the National Biomedical ESR Center: Saturation Recovery apparatus at S-band (3 GHz) became operational in May, 1989. Generally speaking, the sensitivity for spin-labeled aqueous systems is about two times less than at X-band, and is considered sufficient for most pulse experiments. An unexpected initial result is that spin label T1's are decreased at S-band by an amount that is, within a few percent, the ratio of microwave frequencies. Whether or not this is mere coincidence or a discovery of a linearly dependent liquid phase spin lattice relaxation time will require experiments at other frequencies. It is planned to build loop gap resonators for saturation recovery at several frequencies within the octave bandwidth of the S-band bridge to address this question.

Pulse saturation recovery apparatus at 19 GHz is nearly finished. We look forward soon to having a true multifrequency saturation recovery capability at 2, 3, 4, 9.5, and 19 GHz.

From the IERC in Urbana: *W-Band Spectrometer:* The new W-band (94 GHz) spectrometer, which incorporates a superconducting magnet, is now in limited operation. In the current configuration, both solid and liquid samples are accommodated in 0.7 mm o.d. fused quartz tubes. Radicals near g = 2 are now being studied over a range 33.5 ± 0.014T with room-temperature sweep coils under computer control. A brief description of the spectrometer will be given at the 31st Rocky Mountain Conference in Denver (August 3, 1989) and printed in a resulting symposium volume. While this system is still under development and thus is not yet a regular user facility, it is now possible to discuss prospective collaborative experiments with outside investigators. Contact Linn Belford or Bob Clarkson.

Software: As a service to users, IERC makes available without charge some of its software (e.g., QPOW and certain other programs to simulate powder EPR spectra of anisotropic systems as well as DATAPG and DATAEG, programs to display and manipulate spectra on IBM-PC-compatible computers with PGA or EGA monitors). IERC will no longer distribute EPRWARE (see the notice at the end of this Newsletter).

From the Biotechnology Resource in Pulsed EPR in New York: This Resource (Prof. Jack Peisach, Director) has produced a new edition of "PULSED EPR SPECTROMETERS" (85pp., March, 1989). This booklet is a directory of pulsed EPR spectrometers in 37 laboratories around the world. Data are given for spectrometers at the following locations. In FRG: Univ. Dortmund (K. P. Dinse); Homburg/Saar, Univ. des Saarlands (J.

Hüttermann); Karlsruhe, Bruker GMBH (D. Schmalbein); Univ. Stuttgart (M. Mehring). In France: Marseille, Lab. Electr. des Milieux Cond. (J.-P. Gayda). In GDR: Leipzig, Karl-Marx Univ. (W. Windsch, G. Volkel, and W. Brunner). In India: Univ. Hyderabad (P. A. Narayana). In Israel: Rehovot, Weizmann Inst. (D. Goldfarb). In Japan: Osaka Univ. (K. Kuwata); Sapporo, Hokkaido Univ. (T. Ichikawa). In the Netherlands: Univ. Leiden (J. Schmidt); Univ. Nijmegen (E. J. Reijerse and A. A. K. Klaassen). In Sweden: Linkoping Univ. (A. Lund and J. Westerling). In Switzerland: Zürich, ETH-Center (A. Schweiger). In USA: Albany, NY, SUNY (C. P. Scholes); Annandale, NY, Exxon (H. Thomann); Argonne, IL, Argonne Nat'l Lab., IL (M. K. Bowman and J. R. Norris; also A. P. Trifunac); Berkeley, CA, Univ. Calif. (M. P. Klein and D. Britt); Binghamton, NY, SUNY (D. C. Doetschman); Boston, MA, Northeastern Univ. (R. LoBrutto); Bronx, NY, Albert Einstein Coll. Med. (J. Peisach and J. McCracken); Cambridge, MA, MIT (W. H. Orme-Johnson); Chapel Hill, NC, UNC (L. G. Rowan); Univ. Denver, CO, (G. R. Eaton); Univ. Houston, TX (L. Kevan); Ithaca, NY, Cornell Univ. (J. H. Freed); Los Angeles, CA, USC (L. R. Dalton); St. Louis, MO (McDonnell Douglas Corp.); St. Louis, MO, Washington Univ. (T. T. Lin); Urbana, IL, Univ. of Ill. (R. L. Belford and R. B. Clarkson). In USSR: Kazan State Univ. (I. Kurkin and V. Shlenkin); Kazan, Phys. Tech. Inst. of USSR Acad. Sci. (E. Kharakhashian); Leningrad, Ioffe Phys.-Tech. Inst. (M. Petrov and M. Shliagin); Moscow, USSR Acad. Sci. (Ya. S. Lebedev); Moscow, Karpov Phys. Chem. Inst. (V. Milinchuk); Novosibirsk, USSR Acad. Sci., Siberian Branch (Yu. D. Tsvetkov). For each spectrometer, the booklet gives technical specifications, an indication of the types of experiments for which it is used, and other comments. Those interested in this edition or in having their pulsed spectrometers listed in future editions are invited to contact Dr. Peisach at the Biotechnology Resource in Pulsed EPR Spectroscopy (address above).

ANNOUNCEMENT: ***L.I.V.E.R.S., a new NIH Research Resource at Columbus:*** The Laboratory for *In Vivo* Electron Spin Resonance Spectroscopy, "L.I.V.E.R.S.," at the Ohio State University is an NIH research resources development program headed by Prof. Lawrence J. Berliner, Department of Chemistry, 120 W. 18th Avenue, Columbus, Ohio 42310-1173, USA. Telephone (614) 292-0134. The L.I.V.E.R.S. center has currently available three Varian E-line instruments, one E-12, one E-9, and V-4502 12-inch magnet system with an up-to-date Mark II field controller. In addition, a homemade L-band solenoid magnet system (30 cm diameter) is available, as well as an E-4. In addition, the Department of Chemistry has recently acquired a Bruker ESP-300 which, while not generally available, may be used under special circumstances. The laboratory is set up for *in vivo* ESR L-band investigations using flat loop surface coils, loop gap resonators, and reentrant cavity resonators. Furthermore, imaging capabilities have been developed at L-band with the single loop surface coil and it is hoped that within the next year imaging will be feasible with the higher sensitivity loop gap and reentrant cavity resonators. It should be emphasized that L.I.V.E.R.S. is not a full NIH Center, but a resource development which proposes to become a Center in the next three to five years. Therefore, our service capabilities are not up to the potentials of the Urbana, Milwaukee, or New York Centers. Nonetheless, we welcome any collaborations in the area of low-field ESR on small animals using nitroxides, spin traps, or naturally occurring free radicals.

SOFTWARE FOR ESR SPECTROSCOPY

by Richard Cammack
Biochemistry Section
Division of Biomolecular Sciences
King's College, Campden Hill Rd
London W8 7AH, U.K.

Computers greatly enhance the power of ESR spectrometers through capabilities such as signal averaging, spectrum subtraction, integration, and data storage. They are now standard accessories on new instruments. Probably most of the spectrometers now in operation have been equipped with some kind of computer. This has been done with many different types of interfaces to many different types of computer. However, computers are rapidly developing and may become obsolete before the spectrometers do. One area where users can usefully exchange information is therefore the interfacing of spectrometers to more commonly available microcomputers and the software for data collection, manipulation, and storage.

Another area of general application is the analysis and simulation of spectra. Here again, many programs have been written for special applications. These include isotropic spectra of radicals in solution with hyperfine interactions; spectra and rotational diagrams of single-crystal samples; powder spectra of anisotropic solid samples; and spectra of spin labels in motion.

Computers have become considerably cheaper and more powerful over the years; it is now possible to use readily-available microcomputers to carry out many of the computations that until recently required a mainframe. Meanwhile, the larger computers now can carry out more extensive computations in a shorter time. A great deal of software already has been written by users for various applications; this activity has been uncoordinated. Software is also being written by the spectrometer manufacturers, principally concerned with spectrum acquisition, storage, and display, may be of interest even to users of older equipment if it sets *de facto* standards for storage and transmission of spectra.

Users have tended to write specialty programs for their own applications. While this seems a wasteful duplication of effort, it was done because of high hardware costs, incompatibility between computer systems, and poor information exchange. Now that so much software has been written, it should be possible to adapt many existing programs to other computers, e.g., with the aid of standard library routines.

The ESR Group of the Royal Society of Chemistry, with its regular meetings, seems to be a suitable forum for the exchange of information about software. Spectroscopists who have written programs and those who would like to apply software written by others could share information in an ESR Software Users' Group. Its functions would include:

Information exchange on (1) programs for ESR on standard computers, (2) computational algorithms, and (3) interfacing spectrometers to computers.

Standardization of (1) hardware, (2) operating systems, (3) computer languages for programs, and (4) formats for storage and transfer of spectra.

Improving access to existing software by (1) documentation, (2) converting software formats between systems, (3) standard user interfaces, and (4) software maintenance, e.g., fixing bugs, improving, and enhancing.

Communication with other groups, e.g., (1) other ESR spectroscopy groups, (2) other types of spectroscopy groups (e.g., NMR, FTIR), and (3) spectrometer manufacturers.

Organization of further meetings and software swapshops, which might be included in future ESR Group meetings.

Meeting Report: The first meeting on Computers in ESR Spectroscopy and software swapshop was held on April 14, 1989 at the end of the meeting of the ESR Group of the Royal Society of Chemistry at Sheffield, U.K. This lively session provided an opportunity for the exchange of information about available and desired software. Several programs were demonstrated on microcomputers and were available for exchange on diskettes. There were talks on other software and on algorithms for treating various types of problems.

A list was compiled of programs available including free programs provided by members of the ESR Group, some commercially-available software, and some general sources of user-written programs for spectroscopy. This list should be maintained and expanded; it might develop into a generally-accessible list such as a computer Bulletin Board to which users could contribute information directly on programs, updates, documentation, and hardware developments and where they could ask for help on specific problems.

In preparation for another software session, to be held in conjunction with the next Meeting of the ESR Group (March 26-30, Egham), those interested should send information and ideas to R. Cammack (address above; phone 01-937 5411 Ext 264), from whom specific information from the April, 1989 session also may be obtained.

SPIN TRAPPING LITERATURE DATABASE

by Anson S. W. Li
Laboratory of Molecular Biophysics
National Institute of Environmental
Health Sciences, P.O. Box 1233
Research Triangle Park, NC 27709

Spin trapping is a powerful yet convenient technique for the study of free radical reactions. Highly reactive free radicals are detected by reaction with a diamagnetic molecule (usually a nitrone or nitroso compound) to form more stable free radicals (spin adducts) that can be observed by conventional ESR spectroscopy. Since its inception in the late '60's, spin trapping has gained wide acceptance in various fields and is no longer limited to only research chemists. The breadth of applications ranges from clinical studies to high energy physics. Over 1500 references to the technique are listed in Chemical Abstracts. The chore of manually searching a vast amount of printed information warrants the use of a computer.

We have designed a stand-alone database with auto evaluation feature for literature information relating to spin trapping and have implemented it on an IBM PC/AT. The package, including the spin trapping files and the accompanying program, STBDII, is standalone - i.e, does not require extra "add-ons." It is powerful yet user-friendly; command structure is similar to the familiar 1-2-3 light-bar menu; search strategy employs the method of Query-By-Example (QBE); logical combination of any fields is accomplished with AND, OR, NOR, and EXCEPT.

Presently, STDBII (4.0) contains compiled literature files for 5,5-dimethyl pyrrolidine-N-oxide (DMPO), alpha-phenyl-N-tert-butyl nitrone (PBN), 2-methyl-2-nitrosopropane (MNP), alpha-(4-pyridyl-1-oxide) N-tert-butyl nitrone (POBN), nitrosodurene (ND) and 3,5-dibromo-nitrosobenzene sulfonate (DBNBS). A number of less popular traps are included under Weird (all others). Our goal is to incorporate all published work relating to spin trapping. The database files now have over 1100 references with over 2500 entries on parameters alone. Each STDBII file contains information on spin trap used, radical trapped, hyperfine splittings, g-value, a terse summary on the experiment, full bibliographic data and retractions on anything by the author.

Since the demonstration of our STDBII in 1987 (The 19th Annual Southeastern Magnetic Conference, 1987) and its subsequent publication (Anson S.W. Li, Kiran B. Cummings, H. Peter Roethling, Garry R. Buettner, and Colin F. Chignell: J. Magn. Reson., 79:140-2(1988)), we have already shipped over 30 copies to laboratories around the world. Users report STDBII serves well in the following capacities: 1) in identifying spin adducts from the sometimes unique hyperfine splitting parameters; the autoevaluation feature has proved to be very useful, 2) as a key to the spin trapping literature through perusal of the reference section, 3) as a vehicle to retract published wrong assignments.

STDBII is available upon request. The package includes a user manual which lists all the compiled information on spin trapping. Scientists who do not presently own a personal computer could also benefit from browsing through the compilation.

UPDATES AND REQUESTS

UPDATE - NEW ESR SOCIETY: *Announcement by H. M. Swartz. In our last Newsletter we proposed establishment of an ESR society. The many responses to the questionnaire included in that Newsletter were overwhelmingly favorable. Respondents are thanked for several good suggestions. Subsequent discussions among several scientists prominent in EPR have resulted in a decision to proceed with establishment of such a society. The initial organizational meeting will be held at Denver during the 12th Annual International EPR Symposium (July 30-August 3, 1989). About a third of the membership of the steering committee will be determined then.*

This society is to be international. It is to cooperate, not compete, with established ESR organizations such as the ESR Group of the Royal Society.

The next Newsletter will report on the organizational meeting and will solicit suggestions for other members.

NOTICE - EPRWARE UPDATE: *The EPRWARE software package is no longer being distributed directly by IERC. Scientific Software Services (SSS), 305 E. Locust, Bloomington, IL 61701, USA (309-829-9257) is now marketing an updated and enhanced version of this program for EPR data acquisition (IBM-compatible PC with Varian or Bruker spectrometer), storage, display, manipulation (baseline adjustments, scaling, comparison, subtraction, smoothing, integration), and plotting. Source code and phone support are included; help with installation and customization for special applications can be arranged. Contact Dr. Philip D. Morse, II at SSS for information. Users of the original versions, obtained from IERC, may contact either IERC or SSS for help.*

REQUEST FOR INFORMATION ON ASYST SOFTWARE: *Roger Isaacson (Physics Department, University of California at San Diego, La Jolla, CA 92093, USA; Phone 619/534-2505; FAX 619/534-0173; E-mail risaacson@ucsd.BITNET), a new user of the ASYST PC software system, would like to hear from anyone who has ASYST routines suitable for EPR and ENDOR - e.g., efficient normalized signal averaging, averaging, dual monitoring with real time data viewing, fast output to analog xy plotter. The laboratory at La Jolla is trying slowly to phase out the Nicolet 1180, but Isaacson suspects that it will not be easy to reproduce all of its capabilities on a PC. Information received will be shared with others through this column and through the ESR software initiative of the ESR Group in the United Kingdom (see article by R. Cammack above).*