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EPR NEWSLETTER

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From the Editor—

In this issue, with the enthusiastic initiative and assistance of Jim Norris and John Pilbrow, President and Secretary, respectively, of the International EPR Society, we continue our campaign to provide for our readers informative citations and news of all significant awards and honors received by IES members and of awards made by the IES and other organizations in the general area of electron magnetic resonance. It is my hope that Newsletter readers feel well served by publication of these citations, which serve to document the extremely high quality of the awardees chosen by our awards committees. The 1998 IES awardees are cited and honored in this issue, I'm especially pleased that this issue carries a citation for Illinois' own Alex Smirnov as the IES Young Investigator of 1998. On another personal note, I'm equally delighted that the Awards Committee chose to honor as IES Fellows both Charlie Slichter and John Weil. Charlie has been a much-admired University of Illinois fixture ever since he was my beginning physics teacher in 1950, and John has been closely associated with us and has spent considerable time on our campus over the years. Both have made seminal contributions to the development of magnetic resonance sciences, and we've been privileged in our local associations with both of them.

From now on, all nominations for IES awards must include brief citations that would be appropriate for delivery at the award ceremonies and for publication in the EPR Newsletter. Although not mandatory, it would be helpful to include a photograph of the nominee suitable for publication. Instructions and deadlines for making Year 2000 award nominations will be published in the EPR Newsletter later this year. In the meantime, it's not too soon to be thinking of possible candidates for nomination.

As always, we invite comments and suggestions about Newsletter content and especially, submissions of relevant news items and other appropriate material for publication here.

Linn Belford

1998 IES AWARD WINNERS

GOLD MEDAL TO PROFESSOR ARTHUR SCHWEIGER, ETH, ZURICH

Professor Arthur Schweiger, who has spent his entire career at the Swiss Federal Institute of Technology in Zurich is recognised as one of the outstanding leaders in the field of EPR spectroscopy. During the past 15 years or so he and his group have set benchmarks in pulsed EPR spectroscopy through the introduction of novel pulse sequences, bringing to EPR spectroscopy new 1D and 2D methods along the lines of those well established in NMR. This has required both high level interpretive skills and novel designs for probeheads and other dedicated equipment. Contributions to ENDOR studies of a wide variety of substances and novel

Jim Norris (left) presenting the 1998 IES Gold Medal to Art Schweiger in Berlin, August 1998.

methods for site selectivity in CW EPR carried out earlier in his career have been equally outstanding. Much of his work has been motivated by the desire to improve the methods for elucidating hyperfine structure in EPR spectroscopy. Arthur

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Schweiger's work has been recognised elsewhere through being awarded the Zavoisky Prize in 1993 and the Bruker Prize of the Royal Society of Chemistry in the UK in 1994.

Presented by Professor Jim Norris, President of the Society, at the 29th AMPÉRE - 13th ISMAR International Conference, Berlin, Wednesday 5th August 1998.

SILVER MEDAL for PHYSICS and INSTRUMENTATION to DR. BILL MIMS, FORMERLY of the BELL TELEPHONE LABORATORIES

Dr. Bill Mims, in a long and distinguished career at Bell Telephone Laboratories, has contributed enormously to the field of EPR spectroscopy. Yet of the many fine contributions he made through the years, his pioneering developments in pulsed EPR spectroscopy leading to 1D and 2D forms of Electron Spin Echo Envelope Modulation (ESEEM) will long be regarded as his most important scientific achievement. Bill's two outstanding theoretical papers published in 1972 are classics for they made the theory of ESEEM accessible to subsequent generations of EPR researchers. In collaboration with Professor Jack Peisach, he ensured that ESEEM would become a standard method for studies of metal proteins. What is perhaps less well known are Bill's contributions to linear electric field effect (or LEFE) EPR spectroscopy, important in distinguishing between centro-symmetric and non-centro-symmetric sites. His text, *The Linear Electric Field Effect in Paramagnetic Resonance,* is a gem and an impressive exposition of a relatively unfamiliar field, in which he pioneered the application of pulsed methods. Before embarking on ESEEM spectroscopy, much of Bill's earlier work concerned pulsed ENDOR. In awarding the 1998 Silver Medal of The International EPR Society in the Physics/Instrumentation Category to Bill Mims, we are honouring a truly genuine pioneer.

Award to be presented during the 22nd International EPR Symposium in Denver 1999.

SILVER MEDAL for CHEMISTRY to PROFESSOR DICK FESSENDEN of NOTRE DAME UNIVERSITY

The 1998 IES Silver Medal for Chemistry is awarded to Professor Richard Fessenden of Notre Dame University in the USA for his outstanding contributions to the development of EPR spectroscopy as the most sensitive structural and kinetic tool for the characterisation of short-lived organic free radicals in solution. His benchmark paper (with Schuler) in 1963 set new standards for the radiolytic generation of free radicals and for the detailed analysis of hyperfine splittings - of planar and bent alkyl radicals, vinyl and subsequently phenyl radicals. This and subsequent work on photogeneration and polarisation clearly underpins the development of our understanding and application of the CIDNP and CIDEP techniques in chemistry. Dick Fessenden's research career began in NMR for his PhD at MIT. He changed to EPR at Caltech in the late 1950's, subsequently moving to the Mellon Institute and then in 1976 to Notre Dame University.

John Pilbrow (left) presenting the Silver Medal for Chemistry to Dick Fessenden in Berlin, August 1998.

Presented by Professor John Pilbrow, Secretary of the Society, at the 29th AMPÈRE - 13th ISMAR International Conference, Berlin, Wednesday 5th August, 1998.

SILVER MEDAL for BIOLOGY/MEDICINE to PROFESSOR ED JANZEN, UNIVERSITY of GUELPH and the OKLAHOMA MEDICAL RESEARCH FOUNDATION

Edward G Janzen receives the 1998 Silver Medal In Biology & Medicine for his contributions to the development of spin-trapping in biological systems. His publication in 1969 with his student Barry Blackman at the University of Georgia introduced this powerful technique and a subsequent key review article in Accounts of Chemical Research on this subject encouraged numerous EPR spectroscopists to consider using this powerful technique. The application of Spin Trapping, especially with the nitrones DMPO and PBN, to Chemistry, Biology, and Medicine subsequently led to extensive insight into many aspects of free radical chemistry and, as a consequence, thousands of publications by hundreds of authors. Ed Janzen spent much of his career as Chairman of the Department of Chemistry & Biology at the University of Guelph in Canada and in 1990, with Paul McCay, Lee Poyer, and Robert Floyd, he established an NIH-supported Center at the Oklahoma Medical Research Foundation which further expanded the knowledge of the technique throughout the biomedical community as well as making important further advances in its applicability.

Presentation in person was not possible in 1998.

YOUNG INVESTIGATOR AWARD to DR. ALEX SMIRNOV, of the ILLINOIS EPR RESEARCH CENTER

A native of Russia and now a resident of the United States, Dr. Alex Smirnov has made outstanding contributions

Alex Smirnov (left) receiving the 1998 IES Young Investigator Award from John Pilbrow in Denver.

to the international EPR community through both excellence in his own research and collaborative assistance to many colleagues. His introduction of convolution-based simulation and optimization techniques for inhomogeneously broadened EPR spectra and their highly successful use to elucidate dynamics and spin-spin interactions, including CW EPR oximetry in membranes, is exemplary as is his role in extending high-field EPR experiments to aqueous solutions of spin-labeled biomolecules and paramagnetic metal ions. His 50 research publications and 100 research presentations, covering his career from graduate study with the late Professor Lebedev in Moscow to his present appointment as Research Assistant Professor and Laboratory manager of the Illinois EPR Research Center, attest to the quality and versatility of his contributions to EPR science and its applications.

Presented by Professor John Pilbrow, Secretary of the Society during the 21st International EPR Symposium, Denver, Monday 26th July and again by Professor Jim Norris, President of the Society at the 29th AMPÈRE - 13th ISMAR International Conference, Berlin, Friday 7th August.

1998 IES FELLOWS

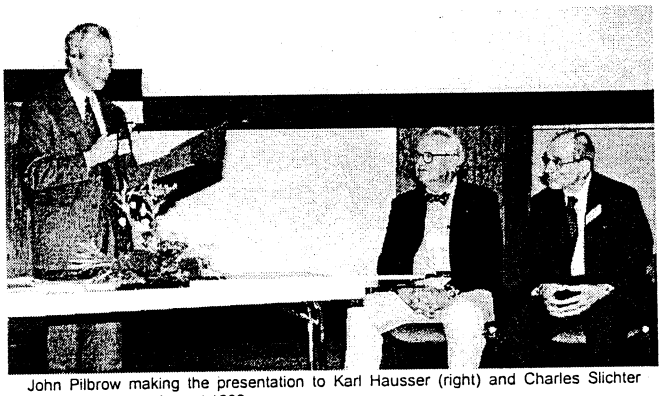
PROFESSOR GEORGE FRAENKEL

George Fraenkel's Fellowship honors his pioneering work in the early development of ESR in chemistry. His extensive ESR studies of organic free radicals in solution included his confirmation of the electronic structure of aromatic radicals in terms of molecular orbital theories, the general validity of the McConnell relation relating unpaired electron density on an aromatic carbon atom to the hyperfine splitting of a proton, and extension of this relation to ^{13}C atom and hetero-atom hyperfine splitting. He developed general spin relaxation theories for organic free radicals in solution, explaining variations in linewidth and T_1 for the different hyperfine lines in terms of correlated modulation of the magnetic tensor parameters by the diffusive molecular motion in the liquid state.

Professor Fraenkel spent his professional career in the Chemistry Department, Columbia University though he is now retired.

PROFESSOR KARL HAUSSER

Karl Hermann Hausser was one of the most influential pioneers in Magnetic Resonance in the Germany of the fifties, a period in which international contacts for German scientists were severely limited. His work on high resolution EPR of free radicals with a record 17 mG linewidth in the early sixties, and soon afterwards the first paramagnetic NMR in organic free radicals in solution, are prominent examples in his early career. He built up strong and well recognized Magnetic Resonances Laboratories both at the Euratom-Center in Ispra and the Molecular Physics Department at the Max Planck Institute in Heidelberg with major achievements in Magnetic Resonance methodology as well as in basic science covering the whole range of Chemical Physics and expanding into applications as far as Medical Imaging. Equally outstanding are his unceasing efforts and inspiring example to foster international contacts. He was President of the Groupement Ampère from 1980-92 and recently served as Vice-President of the International EPR society. In honouring Karl Hausser with Fellowship of the International EPR Society, we are both thanking and acknowledging one of the true pioneers.



John Pilbrow making the presentation to Karl Hausser (right) and Charles Slichter (seated) in Berlin, August 1998.

Presented by Professor John Pilbrow, Secretary of the Society at the 29th AMPÈRE - 14th ISMAR International Conference, Berlin, Wednesday 5th August, Berlin.

PROFESSOR CHARLES SLICHTER

Professor Charles Slichter has been involved in magnetic resonance for more than 50 years, having begun his research at Harvard in the late 1940's. Although most of his research effort has been in NMR, he has made many key contributions to EPR theory and practice. For example, it was the Slichter group that offered the first explanation of the g = 4.3 line due to Fe^{3+} in silicate glass. Early on, he saw the opportunity to apply ENDOR to the study of defects in insulating crystals, with pioneering work on F-centres in alkali halides and the very interesting cubic Fe^{3+} spectrum in silver chloride being amongst the early successes. Charles Slichter's book,

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"*Principles of Magnetic Resonance,*" first published in 1963, provided many important insights into magnetic resonance which were not fully appreciated in EPR until the early 1980's. Since 1950 he has been at the University of Illinois. In appointing Charles Slichter to Fellowship of the International EPR Society, we are honouring an elder statesman of magnetic resonance for the impact his work has had on fundamental issues of importance in EPR.

Presented by Professor John Pilbrow, Secretary of the Society at the 29th AMPÈRE - 13th ISMAR International Conference, Berlin, Wednesday 5th August, 1998.

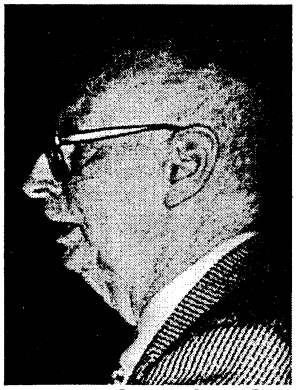
PROFESSOR YURI MOLIN

In 1958 Professor Yuri Molin carried out ESR spectroscopy under an accelerator electron beam in the then Soviet Union while still a student of V.V. Voevodsky in Moscow. This led to many valuable contributions in radiation and photochemistry applications of ESR. In 1961, he moved with Voevodsky to Novosibirsk where he studied spin exchange between complexes and free radicals using EPR, work that later led to his Doctors Thesis in 1971 and a monograph in 1980 "Spin Exchange" published by Springer Verlag. In 1972, he and his colleagues were the first to observe magnetic field effects in radical recombination in solution. More recent work includes Optically Detected EPR to study short-lived spin-correlated radical ion pairs in irradiated solutions and quantum beats in fluorescence resulting from recombination of these pairs. He is one of the founders of spin chemistry, is the author of a great many research papers and several books on ESR and its applications. Since 1981 he has been a Full Member of the Russian Academy of Sciences (formerly USSR Academy of Sciences). Professor Molin is Head of the Fast Reactions Laboratory, Novosibirsk State University.

Presentation on behalf of the Society made by Professor Yuri Tsvetkov, IES Council Member, Novosibirsk, August 1998.

PROFESSOR CHARLES P. POOLE JR.

Professor Charles Poole has been involved in EPR spectroscopy for more than 40 years and is perhaps best known for his book "*Electron Spin Resonance*" published in 1967. This book and the second edition of 1982 have been used as encyclopedias for spectrometer design principles by many EPR researchers. "*Electron Spin Resonance*" is the major review of the performance of all of the early spectrometers in EPR and for that reason will remain a significant source of EPR history. With H.A. Farach and others he has contributed a further four books relating to EPR theory and practice. Charles Poole has carried out significant research using EPR as a tool for studying ferroelectrics and phase transitions in solids in general. He has actively promoted the practice of EPR through conferences in the southeastern region of the USA. For many years Charles edited *Magnetic Resonance Review* and he has been on the Board of the *Bulletin of Magnetic Resonance*. He is currently editing the second volume of the *Handbook of Electron Spin Resonance* to be published by Springer-Verlag later in the year. In honouring Charles Poole with Fellowship of the International EPR Society, we are saying thank you for the many ways in which his work has promoted the cause of EPR spectroscopy.

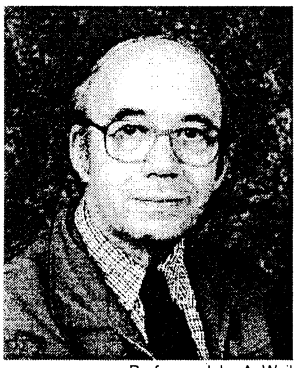

Professor Charles Poole

Professor Poole is an Emeritus Professor of Physics at the University of South Carolina where he spent his professional career after a stint in Industry.

Presented by Professor John Pilbrow, Secretary of the Society during the 21st International EPR Symposium, Denver, Tuesday 27th July.

PROFESSOR JOHN A. WEIL

After a career in EPR spanning close to 50 years at Chicago, Princeton, Argonne National Laboratory and since 1971 at the University of Saskatchewan, Professor John Weil is best known for elucidating the structure of the majority of known magnetic point defects in crystalline quartz. This has involved careful attention to symmetry, or the lack of it, and unusually high-precision measurements. His 1973 treatise with T. Buch and J.E. Clapp, *Crystal Point Group Symmetry and Microscopic Tensor Properties in Magnetic Resonance Spectroscopy*, has provided a necessary and systematic treatment of the relation between crystal (and local) symmetry and EPR (as well as NMR). Seminal contributions are to be found in the early papers with J.H. Anderson – *Determination of the g-Tensor in Paramagnetic Resonance* (1958) and *Direct Field Effects in Electron Paramagnetic Resonance* (1961). Other important contributions include computer simulation software developed since the 1960s in which the nuclear Zeeman term in ligand hyperfine structure was properly included for the first time, the development (together with R. Skinner) of special diagrams to solve spin Hamiltonians, measurements of free radicals in a variety of organic molecules, and investigations of superoxo binuclear cobalt complexes. Recently John Weil shouldered the major share of the revision (1994) of the EPR text by J.E. Wertz and J.R. Bolton. He now holds the position of Emeritus Professor of Chemistry at the University of Saskatchewan, where he continues his research activities.


Professor John A. Weil

In honouring John Weil with a Fellowship of the International EPR Society, we recognize his many outstanding contributions to and strong influence upon the development of EPR spectroscopy and its applications over nearly half a century. We expect yet more important contributions from him in the years to come.

Presentation in person was not possible during 1998.

PROFESSOR DAVID WHIFFEN

A graduate of Oxford, David Whiffen began research in ESR upon appointment as a Lecturer in Chemistry at the University of Birmingham. Whiffen and J.A. Pople established the Basic Physics laboratory at the National Physical Laboratory, largely to entice British scientists back to the UK, and it quickly became an exciting place to work. Under their guidance many notable scientists established their careers, including John Morton, Ray Freeman, FRS, Ray Abraham, Ray Cook, Frank Karasch and Keith McLauchlan, FRS. David was soon elected a Fellow of the Royal Society. David finished his career as Professor of Physical Chemistry at the University of Newcastle. His genius was mainly in analysis, originally applied with unprecedented insight and rigour to radicals trapped in the solid state. Whiffen was the first to show that free radicals generated in single crystals did in fact conform to the symmetry requirements of the host and he realised that the signs of both spin-spin and hyperfine coupling constants could be determined in multiple resonance experiments such as ENDOR. In remembering David Whiffen through appointment to Fellowship of the International EPR Society, we are recognising one of the real pioneers who established a tradition of excellence in the United Kingdom.

Presented in person by Professor Keith McLauchlan, Past-President of the Society, September 1998.

1999 Zavoisky Nominations Invited

The 1999 Zavoisky Award will be presented at the annual Workshop "Modern Development of Magnetic Resonance" in September 1999 in Kazan where E.K. Zavoisky demonstrated EPR in 1944. This prestigious award is given in recognition of an outstanding contribution to the development of electron paramagnetic resonance. 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: B. Bleaney (Oxford), G. Feher (La Jolla), K. Möbius (Berlin), A. Schweiger (Zurich), Yu. D. Tsvetkov (Novosibirsk), and the Chairman K. M. Salikhov (Kazan). The selection of the Awardee is made after consultations with the Advisory Award Committee which comprises: K. H. Hausser (Heidelberg), C. A. Hutchison Jr. (Chicago), and Yu. N. Molin (Novosibirsk). Nominations should be submitted posthaste 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; FAX: 7-8432-765075; E-mail: mosina@dionis.kfti.kcn.ru.

✦ *IES AFFAIRS* ✦

ANNOUNCEMENTS AND REPORTS FROM THE INTERNATIONAL EPR (ESR) SOCIETY

From the Secretary—

I am able to report that Executive Committee Meeting 1/99 was held on Wednesday 17th March at the University of Chicago. Present were the President, Jim Norris, in the Chair, the Secretary, John Pilbrow, the Treasurer, Balaraman Kalyanaraman, and the US Regional Treasurer, Chris Felix in attendance.

Members will be pleased to know that this is the third Executive Committee Meeting that has been held during 1998 and 1999. These meetings have provided valuable opportunities for the Office Bearers to talk face-to-face and to review the overall operation of the Society.

In view of the fact that at the time of the meeting only about one third of members had paid dues for 1998, the Executive Committee agreed to the wording of an email message to be sent to more than 800 members. Criteria were adopted for all IES awards to be made available to the Awards Committees for the 1999 round.

A new awards committee has recently been established for the new Silver Medal for Instrumentation, consisting of Jan Schmidt (Chair), Ron Mason, David Singel and Peter Höfer. A complete listing of the Awards Committees will be provided in the next EPR Newsletter.

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In the next Newsletter we shall introduce a new Society logo.

The Society has been in the embarrassing situation since medals were introduced in 1992 in that only a certificate was awarded to medal winners. The Executive Committee is completing negotiations regarding the production of medals for all previous winners and for future awards.

Revision of the Constitution of the Society has been undertaken in recent months to reflect the practicalities in the operation of the Society's affairs. The final revision agreed to by the Executive Committee will be completed shortly. It will then be re-submitted to the Executive Committee and the Past President. In addition, a number of senior members of the Society who have not been part of the process so far will also be asked to check the revision for logical consistency. When all comments have been taken into account, the revised Constitution, and an Explanatory Memorandum, will be printed in a later Newsletter and members will be asked to vote for its adoption.

The Society has always had provision for affiliation of other societies. The only request so far has come from the Asia-Pacific EPR Society established in January 1997 during the First Asia-Pacific EPR Conference which was held in Hong Kong. On behalf of the Society, The Executive Committee agreed to this request and looks forward to a fruitful relationship over the years with the Asia-Pacific EPR/ESR Society. The Asia-Pacific Society is to hold its second conference late in October in China (advertised elsewhere in this Newsletter).

John Pilbrow
Secretary, International EPR Society

IES Awards —

Previous IES Awards Winners

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

EPR SPECIALIST VIGNETTES

Edited by
Arthur Schweiger

Field-Cycled ENDOR Spectroscopy

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INTRODUCTION

ENDOR spectra of powder samples show inhomogeneous line broadening due to the magnetic inequivalence of otherwise identical spins. The disadvantage of spatial anisotropy in an EPR experiment with disordered samples can partly be overcome in modern high-field EPR [1] with its "single crystal like" spectra. In contrast, the Hamiltonian of Zero-Field EPR (ZFR [2]) contains no terms involving a particular laboratory direction. Yet ZFR is limited to cases of high hyperfine fields or appropriate zero-field splittings on account of sensitivity reasons. If the transitions of interest are excited in zero external magnetic field, and the excitation is detected in a high magnetic field, the high resolution possible in zero field and the sensitivity of X-band EPR are combined. An experiment of this kind called field-cycled ENDOR was proposed by Abragam in 1956 [3], and first performed by Krzystek *et al.* [4] in 1994. The pulsed detection introduced by us [5] extends the general usability of field-cycled ENDOR.

In a field-cycled ENDOR experiment the external magnetic field is switched *adiabatically* from a high

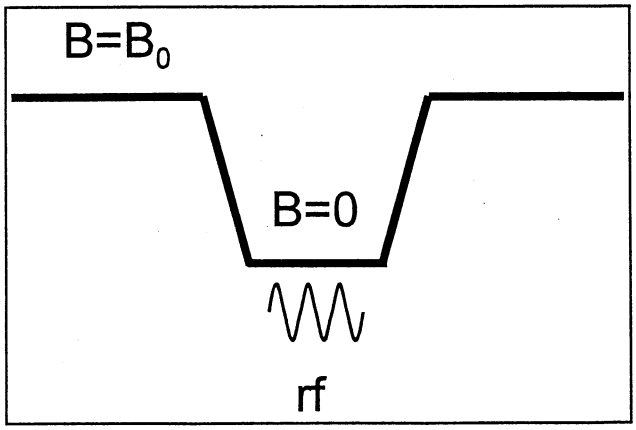

Fig. 1: Principle of a field-cycled ENDOR experiment. The spin system can be excited in zero field with radio-frequency irradiation.

magnetic field $\mathbf{B}_0$ to zero after complete spin relaxation. This results in a reduction of the spin temperature since the entropy of the spin system remains constant on account of the adiabatic transit [6]. In zero field relaxation processes with a time constant T_{1D} can take place, because the temperature of the spin system and the lattice are different. If the magnetic field is restored to $\mathbf{B}_0$ after a time short compared to T_{1D}, the magnetization may return to its original high-field value. Exciting the transitions of interest in zero field with *rf*-irradiation destroys a part of the magnetization. This magnetization change can be observed after the return to high field by a "detector" spin system (Fig. 1).

Experiments of this kind have been known for a long time in NQR double-resonance spectroscopy (*level crossing*, DRLC [7]) in which protons are usually used as detectors for

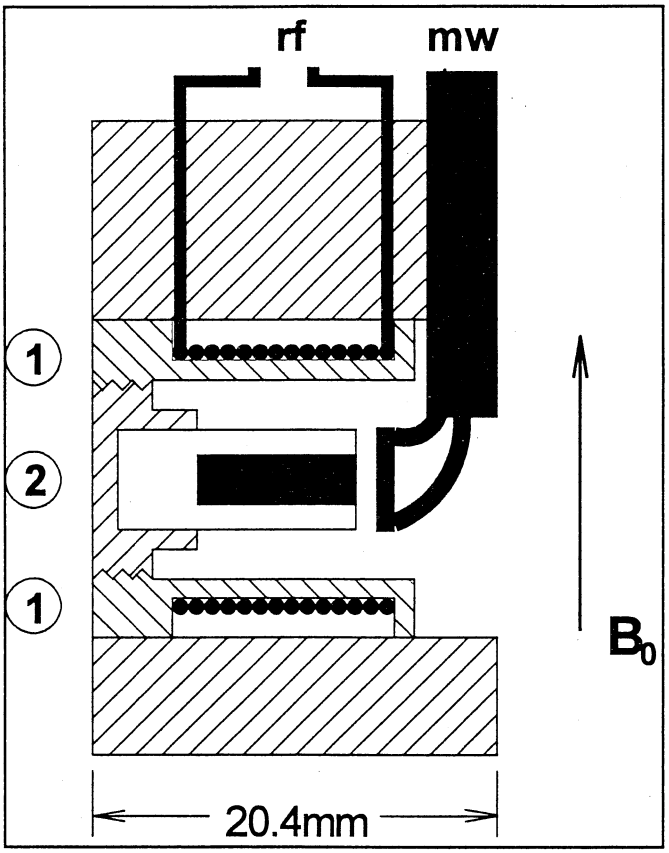

Fig. 2: Probehead for pulsed field-cycled ENDOR. (1) Rexolite ENDOR coil support. (2) Rexolite holder for the bridged loop-gap resonator.

transitions of adjacent quadrupole nuclei. Similarly, in a field-cycled ENDOR experiment, electrons are used as detectors for hyperfine transitions or nuclear quadrupole transitions in zero magnetic field. Two adiabatic conditions must be met: (a) The complete cycle time t_{cyc} must be short compared to the longitudinal high-field and zero-field relaxation times T_1 and T_{1D}, i.e., $t_{cyc} << T_1, T_{1D}$; (b) the switching rate of the magnetic field must fulfill the condition $|\mathbf{B}_0 \times d\mathbf{B}_0/dt|/B_0^2 << \gamma B_0$. For a reversible cycle, this means that field switching must not be too fast. The adiabatic condition (b) is easily satisfied for electrons, but condition (a) can only be met with rapidly switched air-core magnets due to the short electronic spin lattice relaxation times, which are typically a few milliseconds at 4.2 K. Our field-cycling

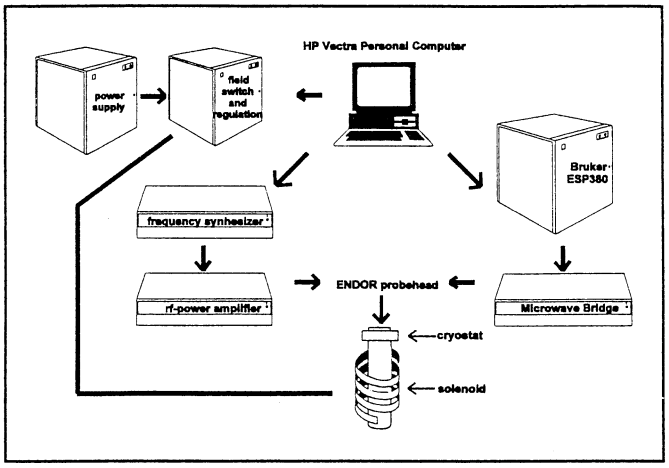

Fig. 3: Principal design of our field-cycled ENDOR spectrometer (see text).

spectrometer [8] can accordingly be switched from 0.33 Tesla to zero within 0.5 ms. The zero-field dwell time must be choosen long enough to ensure ENDOR excitation, and short enough to recover a part of the longitudinal magnetization at the end of the cycle. In the first field-cycled ENDOR experiment of Krzystek, the *cw*-detection of the spin magnetization took 50 ms. Our electron spin echo detection of the magnetization starts immediately after settling of the magnetic field and is finished within 2.5 µs. This is mandatory for substances with rapid high-field relaxation in order to gain information on the magnetization change during the zero-field dwell time.

EXPERIMENTAL

The main part of a *field-cycling* spectrometer is a rapidly switched solenoidal coil into which the tail of a liquid helium cryostat fits. The problems in designing a field-cycled ENDOR probehead are the limited space in the cryostat, and the collinearity of the external magnetic field and the cryostat axis. Therefore, the dimensions of the resonator and of the coupling assembly are critical. Commercially available EPR probeheads cannot be employed. The probehead of Krzystek was a custom-made TE_{102} type cavity. We use a bridged loop gap resonator [9] (Fig. 2) in our experiments because of its small dimensions and its good transparency for radio frequency irradiation. The resonator is handmade by chemical deposition of silver on a quartz glass tube [5]. The probehead includes a 14-turn ENDOR coil which is wound around a cylindrical Rexolite support, and is fixed by a teflon ribbon. The bridged loop gap resonator inside the ENDOR coil is aligned perpendicular to the axis of the field-cycling solenoid, and supported by a movable rexolite holder. Impedance matching is performed at room temperature by rotating the resonator holder which shifts it relative to the coupling loop.

Fig. 3 shows the overall design of our field-cycled ENDOR spectrometer. A personal computer controls the field switch and field regulation unit, the radio-frequency generator, and it triggers a Bruker ESP 380 spectrometer. A 50 W rf power amplifier was used for the ENDOR excitation. The *field switch and regulation unit* is a complicated home built device whose principle is shown in Fig. 4. The current of 510 A flowing through the solenoid S is drawn from a 45 V unregulated power supply and stabilized in a passgate of

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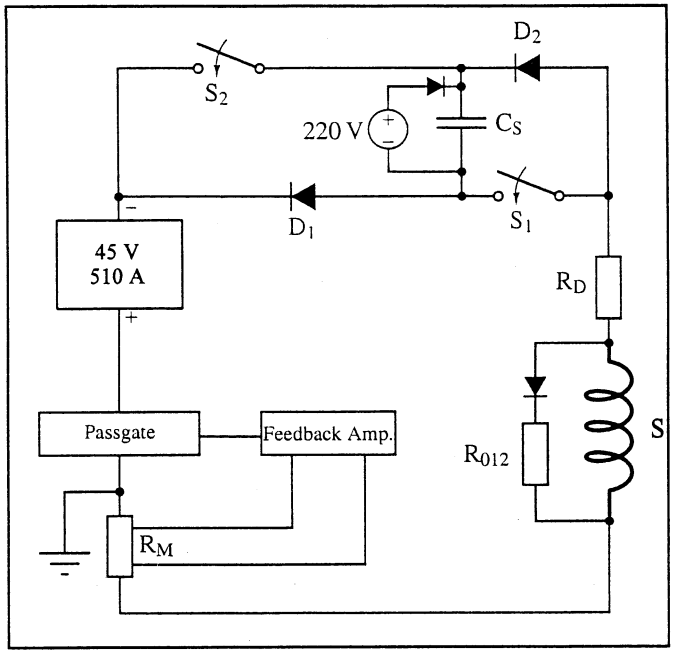


Fig. 4: Field switch and field regulation unit.

120 water-cooled MOSFETs in parallel which are a part of a feedback loop with a current sensing resistor. Darlington transistors are used to switch the current (S_1 closed for high magnetic field, S_2 closed for boosting the return to high field). During the zero-field phase most of the energy of the previously applied magnetic field is stored in the capacitor C_S from which it is drawn to reestablish the magnetic field in the next cycle. A 220 V power supply connected to the capacitor replaces the energy lost during the cycling.

RESULTS AND DISCUSSION

Up to now, there are only two reports of a field-cycled ENDOR experiment: Krzystek *et al.* found deuteron quadrupole transitions in a perdeuterated malonic acid single crystal at 2 K [4] (Fig. 5). The magnetic field was switched off within 1 ms, and the sample was irradiated for 2 ms in zero field. After return to high field and an additional delay of 20 ms the magnetization was detected with 100 kHz field modulation and a sampling time of 50 ms. A strong ENDOR effect of 25 % was found, the same order of magnitude as in high field ENDOR experiments. The two molecules in the unit cell of malonic acid differing in orientation become magnetically equivalent in zero field. Since the pure quadrupole interaction of spin 1 nuclei gives rise to three transitions ν_+, ν_-, and ν_0, twelve lines are expected in the experimental spectrum from the two methylene and the two carboxylate deuterons. The four ν_0-transitions are expected in the frequency region below 20 kHz from previous conventional ENDOR experiments on malonic acid single crystals. The dashed lines in Fig. 5 indicate the ν_+ and ν_- transitions calculated with the quadrupole coupling constants given in Ref. [4]. The transitions b and c actually represent two transitions each. A distant ENDOR mechanism was proposed for this experiment, the energy levels of the deuterons therefore being equivalent to those of molecules in a diamagnetic sample.

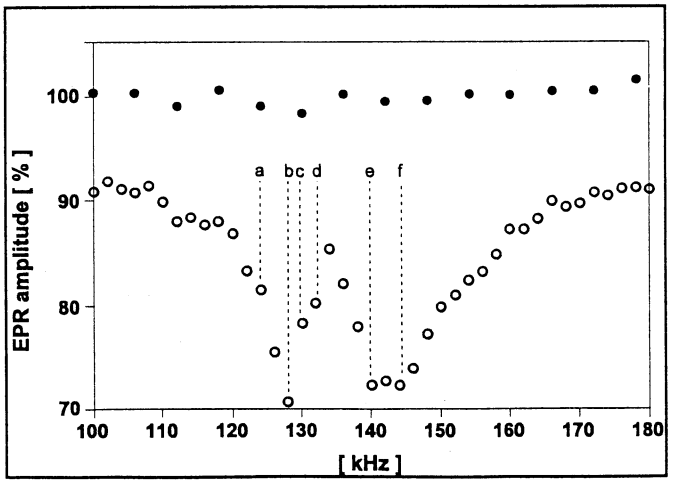


Fig. 5: *cw* field-cycled ENDOR spectrum of an irradiated perdeuterated malonic acid single crystal [4]. (bottom) Recovered EPR signal after irradiation in zero field. 5 accumulations, microwave frequency 9.2 GHz. (top) Reference points obtained without rf irradiation. Irradiation time in zero field was 2 ms. The dashed lines indicate the line positions calculated with the deuteron quadrupole coupling constants given in Ref. [4].

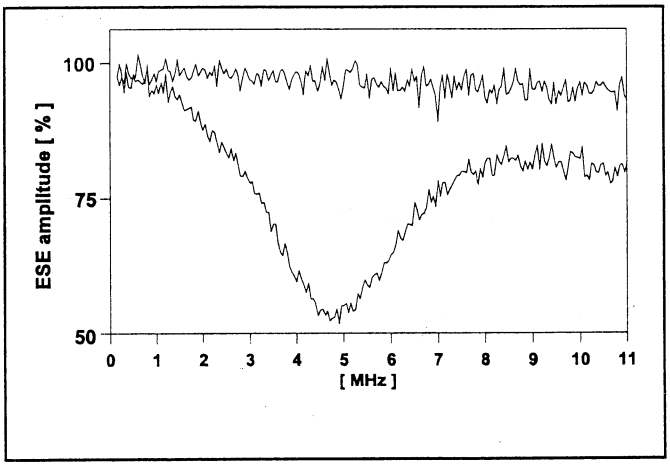


Fig. 6: Pulsed field-cycled ENDOR spectrum of a coal sample. (bottom) Recovered EPR amplitude after irradiation in zero field, no accumulation, microwave frequency 9.3 GHz. The sample was irradiated in zero field for 800 µs. (top) Equal experimental conditions, yet without rf irradiation. Two low-power microwave pulses of 300 ns length were used for the detection.

Fig. 6 (lower trace) shows our pulsed field-cycled ENDOR spectrum of coal (impregnating pitch HL, VfT AG Castrop-Rauxel) at 4.2 K [10]. In zero field the sample was irradiated for 800 µs with a frequency stepped by an equal increment of 50 kHz after each cycle. The echo intensity was monitored 2.5 ms after switching back to high field. Seventy percent of the high-field EPR signal is lost due to spin lattice relaxation in zero field. More of the EPR signal can be recovered by working at lower temperatures. A comparison with the upper trace of Fig. 6, obtained without rf irradiation in zero field, shows the remarkably strong ENDOR effect of 50 %. Only one broad ENDOR line can be seen, similar to the broad powder patterns found in room temperature HYSCORE experiments of the same compound, and assigned to ^{13}C hyperfine couplings [11]. While the experiment of Ref. [4] represents the field-cycled equivalent of a distant ENDOR experiment, the spectrum obtained for coal is the first field-cycled ENDOR spectrum of a nucleus with direct magnetic coupling to the electron spin. In recent experiments performed in our laboratory resolution of the

broad ^{13}C transition was possible at 1.6 K. All six hyperfine transitions expected in zero field for a S=½, I=½ spin system were found.

ACKNOWLEDGEMENT

Financial support from Deutsche Forschungsgemeinschaft is gratefully acknowledged.

REFERENCES

1. Y.S. Lebedev, High-Frequency Continous-Wave Electron Spin Resonance, *in* "Modern Pulsed and Continous-Wave Electron Spin Resonance" (L. Kevan and M.K. Bowman, Eds.), pp. 365-404, J. Wiley, New York (1990).
2. R. Bramley and S.J. Strach, Electron Paramagnetic Resonance Spectroscopy at Zero Magnetic Field, *Chem. Rev.* **98**, 49-82 (1983).
3. A. Abragam, Une nouvelle méthode pour la polarisation des noyaux atomiques, C. R. Acad. Sci. **242**, 1720-1722 (1956).
4. J. Krzystek, M. Notter, and A.L. Kwiram, Field-Cycled Electron Nuclear Double Resonance, *J. Phys. Chem.* **98**, 3559-3561 (1994).
5. G. Sturm, A. Lötz, and J. Voitländer, Pulsed EPR with field-cycling and a bridged-loop-gap resonator made by chemical deposition of silver, *J. Magn. Res.* **127**, 105-108 (1997).
6. C.P. Slichter, *Principles of Magnetic Resonance*, pp. 219-246, Springer, Berlin (1989).
7. D.T. Edmonds, Nuclear Quadrupole Double Resonance, *Phys. Rep.* **29**, 233-290 (1977).
8. J. Olliges, A. Lötz, D. Kilian, and J. Voitländer, Boron nuclear quadrupole couplings and localized electronic wave functions in the boron clusters *o*-carborane and *o*-silaborane, *J. Chem. Phys.* **103**, 9568-9573 (1995).
9. S. Pfenninger, J. Forrer, and A. Schweiger, Bridged loop-gap resonator: A resonant structure for pulsed ESR transparent to high-frequency radiation, *Rev. Sci. Instrum.* **59**, 752-760 (1988).
10. G. Sturm, D. Kilian, A. Lötz, J. Voitländer, Pulsed Field Cycled ENDOR Spectroscopy, Proceedings of the Joint 29th Ampere-13th ISMAR International Conference, Berlin, pp. 216-217, 1998.
11. P. Höfer, Distortion-Free Electron-Spin-Echo Envelope-Modulation Spectra of Disordered Solids Obtained from Two- and Three-Dimensional HYSCORE Experiments, *J. Magn. Res.* **111**, 77-86 (1994).

Building the Perfect Beast

by Chris Bender
bender@spin.aecom.yu.edu

'CORRELATORS' AND ECHO MODULATION SIMULATORS

Correlation theory is a mathematical topic that is related to communication theory and information transfer. It was picked up by engineers from physicists and is related to entropy theory. It boils down to the idea of being able to mathematically describe systems that are comprised of many irregular parts by statistically weighting each part about which some property (i.e. information) is known. In other words, it's a form of statistical mechanics - the maximum entropy and related methods of signal analysis are familiar manifestations in magnetic resonance.[1]

The classic text on correlation theory is by Lange,[2] and in it there are descriptions of high frequency electronic circuits that may be used to study correlation theory and its ramifications. The devices are of general interest to the EPR community because many of the mathematical principles displayed by these circuits are analogous to spin echo modulation, which is merely a form of beat frequency correlation. Lange cites two circuits (Figure 2a and b) that are both based on mixers and delay lines,[3,4] and their typical outputs immediately suggest analogy to an echo modulation trace (Figure 1a and b). One of the characteristics of these traces that made an impression on me is the 'spiky-ness' of the first few oscillations; I often see something similar in echo modulation traces in the first microsecond of data (associated with the so-called 'double quantum' line from ^{14}N).

When I was a graduate student, I taught a lab in which a 'computer' was built in order to simulate chemical reaction kinetics, and from the analogy between electrical and chemical rate laws the student presumably learned the nuances between the mathematical model and chemical reaction kinetics. These two 'correlators' make a good educational system for the modeling of time-domain magnetic resonance and perhaps suggest a novel perspective on describing the dynamics of the spin system.

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

REFERENCES:

1. De Beer, R., D. Van Ormondt, W.W.F. Pijnappel, and J.W.C. Van der Veen, 1988, *Israel J. Chem.*, **1988**, *28*, 249-261.
2. Lange, F. *Correlation Techniques*. Iliffe Books, London 1967.
3. Wilcox, R.M. *Proc. IRE* **1954**, *42*, 1512-1515.

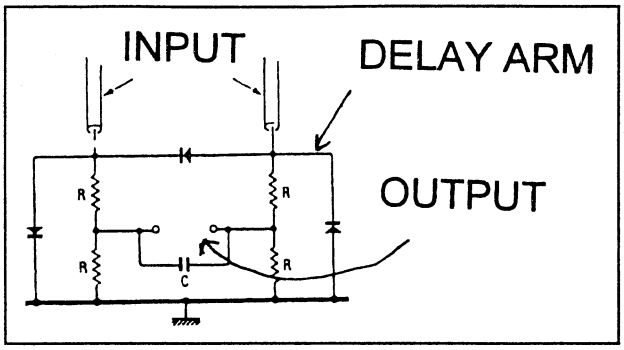


Figure 2a: Circuit schematics for correlators—Wilcox.

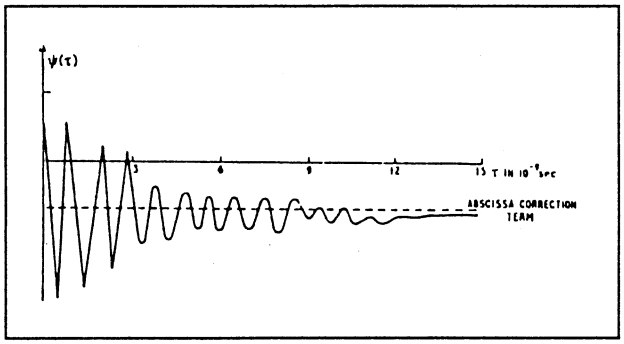


Figure 1a: Correlator response in the time domain—Wilcox.

4. Page, R.M.; Brodzinsky, A.; Zirm, R.R. *Proc. IRE* **1953**, *41*, 128-131.

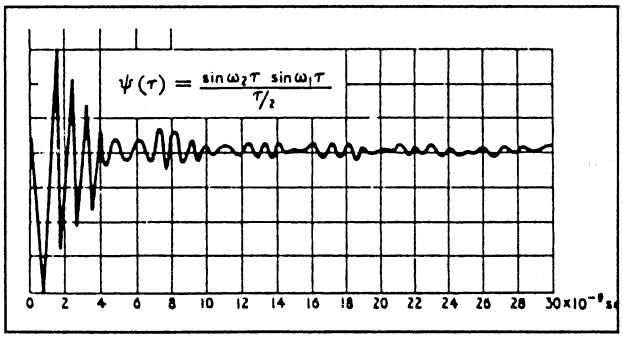


Figure 1b: Correlator response in the time domain—Page, *et al.*

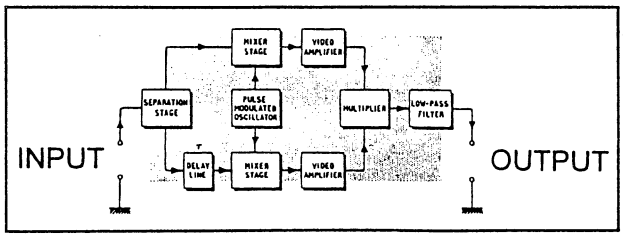


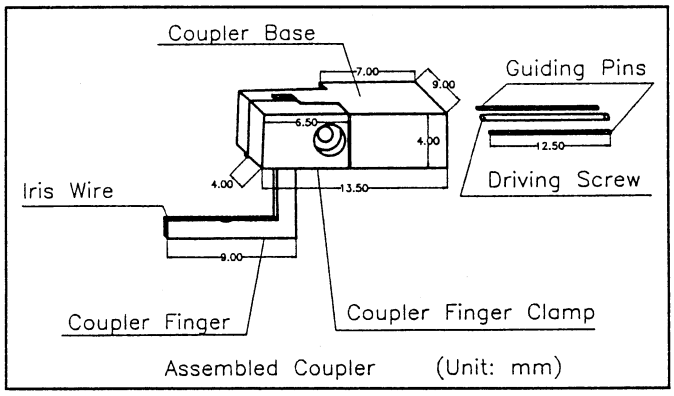
Figure 2b: Circuit schematics for correlators—Page, *et al.*

TIPS & TECHNIQUES

A New Robust Coupler for the Q-band Cylindrical TE_{011} Cavity

Junlong Shao and N. Dennis Chasteen
Department of Chemistry, University of New Hampshire, Durham, NH 03824

The Varian E-110 microwave bridge and the cylindrical TE_{011} cavity are still widely used in Q-band cw-EPR spectroscopy. Hyde and colleagues significantly improved the signal/noise ratio of the Varian Q-band bridge by adding a low-noise GaAs field effect transistor microwave amplifier, a balanced mixer and a Gunn diode oscillator as the microwave source.[1] A robust yet sensitive ribbon-wound TE_{011} cylindrical cavity for Q-band EPR/ENDOR spectroscopy, capable of repeated temperature cycling down to 2 K, was developed by Wang and Chasteen.[2] However, critically coupling of the cavity at low temperature has been a problem because the original Varian coupler frequently breaks when adjusted at low temperature. The difference in the thermal coefficients of expansion of Rexolite and steel causes the threaded Rexolite coupler to grip the steel driving screw at low temperature. When adjusted, the fragile coupler finger tends to rotate laterally against the waveguide and snap.



We have therefore designed a new coupler which is easy to machine, assemble and adjust (see figure). It consists of three parts: a coupler base, coupler finger clamp and coupler finger. The coupler base and coupler finger clamp are made of alloy 360 standard free-cutting brass which is free to magnetization. The coupler finger is made of Rexolite. The small protrusion on the bottom of the coupler base is designed to insert into the slot in the waveguide and guides the precise movement of the coupler base back and forth. The Rexolite finger, if broken, is easily replaced.

The coupler is installed by first prying slightly the two guiding pins on the Varian waveguide and sliding the coupler base onto them. Then the coupler base is pushed slightly to one side and the coupler finger is inserted into the waveguide slot. The coupler base is released and the finger is inserted in the coupler base. Next, the coupler base is pushed toward the cavity. After adjusting the height of the finger so that its tip is centered in the opening at the top of the cavity, the finger is tightened in place by the screw. The positions of the guiding pins differ for some Varian waveguides, so the appropriate dimensions need to

be checked before machining the coupler base. Detailed drawings are available on request. Supported by NIH grant R37 GM20194.

References

1. J. S. Hyde, M. E. Newton, R. A. Strangeway, T. G. Camenisch, and W. Froncisz, *Rev. Sci. Instrum.* 62, 1991, 2969-2975.
2. W. Wang and N. D. Chasteen, *J. Magn. Reson., Series A*, 116, 1995, 237-243.

BOOKS & PROCEEDINGS

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

The Canadian Society for Chemistry has made a number of copies of its volume *Electronic Magnetic Resonance of the Solid State* available to members of the International EPR Society at US$60. At a discount of ⅓ off the regular international price of US$90, this volume will be a handsome and informative addition to your reference collection. Produced in 1987, *Electronic Magnetic Resonance of the Solid State* contains 43 review articles written and refereed by leading authorities in the field. The volume covers most aspects of EPR spectroscopy, ranging from theory through structural studies, multiple resonance techniques and time-resolved spectroscopy to the very latest in EPR imaging.

To order, contact Vicki Campbell, The Chemical Institute of Canada, 130 Slater Street, Suite 550, Ottawa, ON K1P 6E2, CANADA; E-mail: cjche@istar.ca; ☎: 1-613-232-6252 ext. 228.

NOTICES OF MEETINGS

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

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

The 22nd International EPR Symposium will be held in Denver, August 1-5, 1999, at the Hyatt Regency Denver, in conjunction with the 41st annual Rocky Mountain Conference. About 150 people participate in the EPR Symposium each year, presenting over 100 papers. Approximately 1000 people attend the Rocky Mountain Conference, which also includes an NMR Symposium and instrument exhibit. Sunday, August 1st, Bruker Instruments will run a tutorial Workshop on Pulsed EPR at the University of Denver. The EPR Symposium will start Sunday evening with an open house at the University of Denver EPR labs, including refreshments provided by Bruker Instruments. The International EPR Symposium covers all aspects of EPR spectroscopy and contributions in all areas are invited. This year there will be special sessions on electron-electron distance measurements by EPR; in vivo EPR organized by Hal Swartz; and echo envelope modulation recognizing the contributions of Bill Mims, organized by Jack Peisach.

We invite you to participate in the EPR Symposium. Researchers are encouraged to present unpublished results and tentative conclusions to stimulate discussion. We suggest that you consider presentations in the poster sessions, which have proven to be an excellent forum for exchange of ideas.

This year the book of abstracts for the Rocky Mountain Conference will be prepared electronically. Instructions for preparation and submission of an abstract can be found at:

http://www.milestoneshows.com/rmcac

Updated information on the conference, including the preliminary program, is posted on our web page:

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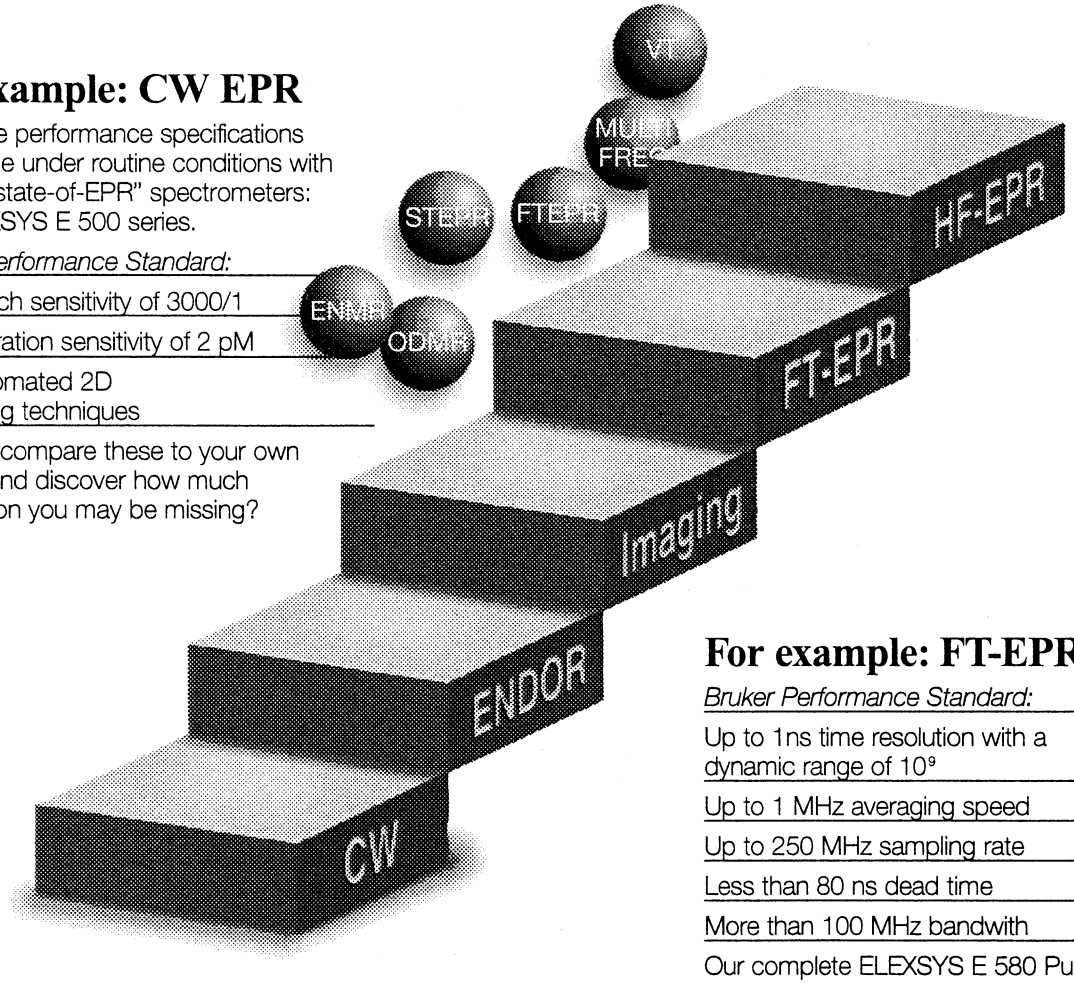

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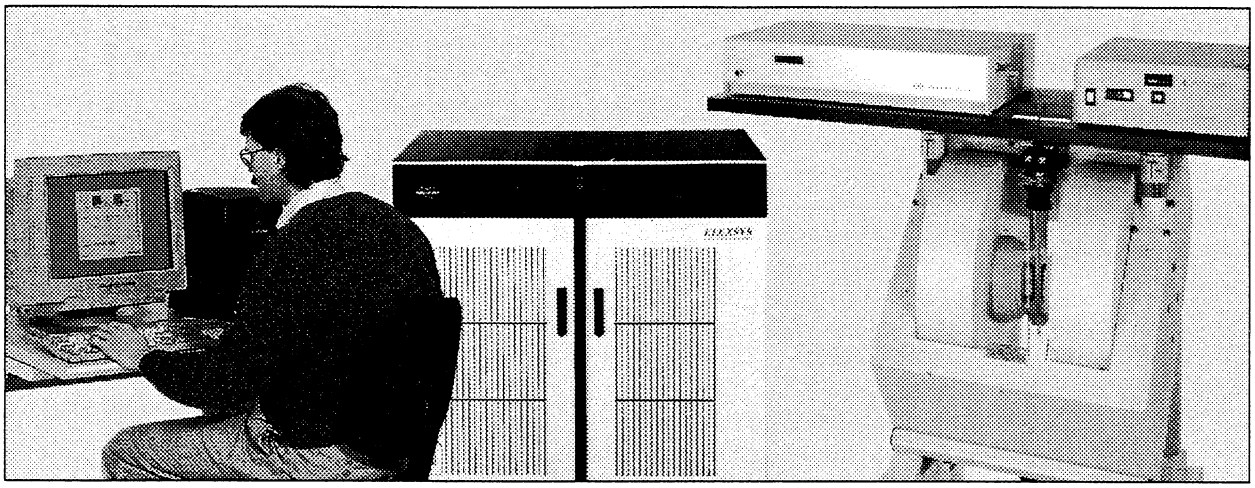

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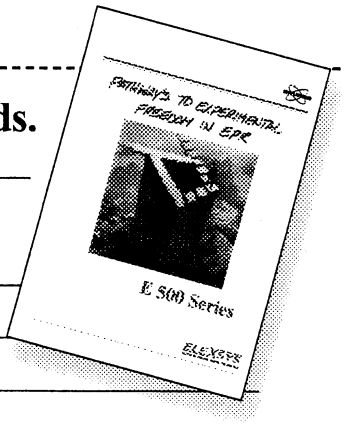

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VI INTERNATIONAL SYMPOSIUM on MAGNETIC FIELD and SPIN EFFECTS in CHEMISTRY and RELATED PHENOMENA, Emmetten, Switzerland, August 21-26, 1999.

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

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

CONFERENCE ON "FREE RADICALS, PARAMAGNETIC CENTERS AND HUMAN DISEASES," Smolensk, Russia, September, 1999.

Requests for more information should be sent no later than April 15, 1999 to the Secretary of the conference: Dr. Vera Podoprigorova, Dept. Internal Medicine, Smolensk State Medical Acad., 28 Tenisheva str., Smolensk, 214019, Russia; Fax: 7-812-558114; E-mail: dnmax@globus.smolensk.ru. Indicate your home and work addresses, fax and E-mail address, and level of participation (oral presentation or poster). Abstracts are requested by April 15. (No more than 1 page, not exceeding 250 words, double-spaced). The fee of US$200 includes hotel, breakfast, lunch, dinner, coffee and tea, conference books and the Social program.

INTERNATIONAL WORKSHOP on TECHNIQUES and BIO-MEDICAL APPLICATIONS of *IN VIVO* EPR and PEDRI, University of Aberdeen, Scotland, UK, September 12-17, 1999.

This will be the next meeting in the "In Vivo EPR" series, which has met in L'Aquila, Yamagata and Dartmouth in recent years. It will cover all aspects of Instrumentation, Techniques and Applications relating to In Vivo EPR, EPR Imaging and PEDRI (Overhauser techniques) in bio-medicine.

Further information and registration details are available on the Workshop website:

http://www.abdn.ac.uk/~mph096/epr99/

Alternatively, if you would like a paper copy sent to you, please contact Dr. David J. Lurie, EPR99 Workshop, Dept. Bio-Medical Physics, Univ. Aberdeen, Foresterhill, Abderdeen AB25 2ZD, UK. E-mail: epr99@biomed.abdn.ac.uk; ☎: 44-1224-663123 (extension 54061); FAX: 44-1224-685645. We hope to see you in Aberdeen in September!

SUMMER SCHOOL on ADVANCED METHODS in EPR: APPLICATIONS to CHEMISTRY, PHYSICS and BIOLOGY, Caorle, Italy, September 12-19, 1999.

A European Summer School on Advanced methods in Electron Paramagnetic Resonance Spectroscopy. Applications to Chemistry, Physics and Biology will be held 12-19 September 1999 in Caorle (Venice), Italy, sponsored by the European Federation of EPR Groups (http://www.cf.ac.uk/esr/fed.html).

The Scientific Committee consists of M. Brustolon (Department of Physical Chemistry, Padova, Italy); C. Corvaja

(Department of Physical Chemistry, Padova, Italy); J.H. Freed (Cornell University, Ithaca, USA); K.A. McLauchlan (Physical & Theoretical Chemistry Laboratory, Oxford, UK); K. Möbius (Freie Universität, Berlin, Germany); K. M. Salikhov (Zavoiski Institut, Kazan, CSI); J. Schmidt (Huygens Laboratory, Leiden University, NL); A. Schweiger (ETH, Zurich, CH); A. Sotgiu (University of L'Aquila, Italy).

The Organizing Committee consists of M. Brustolon (president); D. Carbonera (Padova); C. Corvaja (Padova); A.L. Maniero (Padova); L. Pasimeni (Padova); A. Toffoletti (Padova); U. Segre (Modena); A. Zoleo (Padova); A. Sutera (secretary).

Scientific Program: The school will be held on the theory, instrumentation and applications of all the modern EPR techniques. The program of the lectures contains 8 subjects. A co-ordinator and a group of teachers for each of the subjects will organise the lectures and the activities in the school. Each of the subjects will be presented at an introductory level, then applications to the different fields of Chemistry, Physics and Biology will be described, and finally the state-of-the-art developments will be reported. The list of subjects, co-ordinators and teachers is reported below.

•*Time Resolved CW-EPR.* Coordinator K.A. McLauchlan. Teachers: C. Corvaja, P.J. Hore (Oxford); •*Pulsed EPR.* Coordinator J.H. Freed. Teachers: K.-P. Dinse, (Darmstadt), G. Jeschke, (Mainz), H. Levanon, (Jerusalem); •*ESE and ESEEM.* Coordinator A. Schweiger. Teachers: E.J. Groenen, (Leiden), P. Hofer, (Karlsruhe), G. Jeschke, W. Lubitz, (Berlin), Yu. Tsvetkov, (Novosibirsk)), J.L. Zimmermann, (Saclay); •*High Field EPR.* Coordinator J. Schmidt. Teachers: L.C. Brunel, (Tallahassee), K. Möbius, T. Prisner, (Frankfurt); •*EPR Imaging.* Coordinator A. Sotgiu. Teacher: G. Placidi (L'Aquila); •*Multiple Irradiation EPR (ODMR, ENDOR).* Coordinator K. Möbius. Teachers: M. Brustolon, A. Hoff, (Leiden), P. Hofer, W. Lubitz, A. Schweiger; •*Theoretical Advances.* Coordinator K. Salikhov. Teacher: J.H. Freed; •*Single Molecule Detection.* Coordinator J. Schmidt

Location: The school will be held in Caorle (Venice), at the Hotel Europa (http://www.alfa.it/hotel/europa-touring/). Caorle is an ancient small town on the seaside, with a nice historical medieval centre, and holiday facilities. It is located at 50 Km from Venice, and at 40 Km from the Venice international airport Marco Polo.

Admittance: The number of students admitted to the School will be limited to 80. The selection criteria will aim to favour the participation of young researchers with a previous training in basic magnetic resonance spectroscopy. Immediately after the deadline for the application (31 March 1999) the applicants will be informed on the acceptance for them to attend the School.

Registration fee and accommodation: The registration fee is of Lit. 350000 (180 ECU). Accommodation and living expenses full board (beverages not included) will cost for all the period Lit. 525000 (271 ECU) in double room, and Lit. 630000 (325 ECU) in single room. The number of single rooms is limited.

Grants: The financial support comes from the TMR project (Training and Mobility of Researchers) and from the EU Programme "Co-operation with Third Countries and International Organisations" (INCO). Thanks to this support, the

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School will be able to pay the travel and living expenses for 30-35 young scientists (in general: 35 years or under) from the EU members (Austria, Belgium, Denmark, Finland, France, Germany, Greece, Ireland, Italy, Luxembourg, Netherlands, Portugal, Spain, Sweden, United Kingdom) and associated states (Iceland, Israel, Liechtenstein, Norway), and for approximately 10-12 young scientists from Albania, Bosnia-Herzegovina, Bulgaria, Czech Republic, Estonia, FYR, Macedonia, Hungary, Latvia, Lithuania, Poland, Romania, Slovakia, Slovenia, Armenia, Azerbaijan, Belarus, Georgia, Kazakhstan, Kyrgystan, Moldova, Russia, Tajikistan, Turkmenistan, Ukraine and Uzbekistan. The selection of the students eligible for support will take into account their Curriculum Vitae, and in particular their previous training in basic magnetic resonance spectroscopy.

Please note that the selected researchers may not benefit, for any given expense in connection with participation, from TMR (or INCO) funding at the same time as from any other source. It is however allowable for different expenses to be funded from different sources (e.g. registration fees from one source and travel and accommodation from TMR or INCO).

The forms (Registration Form and in case Grant Application Form) must be sent by mail or E-mail to: Prof. Marina Brustolon, Dipartimento di Chimica Fisica, Via Loredan 2, I-35131 Padova (Italy); E-mail: Brustolon@pdchfi.chfi.unipd.it.

The circular can be found on the WEB page:

http://imoax1.unimo.it/~segre/meeting/ESScirc1.htm

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

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

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

Venue and Date—The Colloque AMPÈRE will take place at Vilnius University and Academy of Sciences (in the Centrum of Vilnius, Capital of Lithuania). It will start on Saturday, September 18, 1999 (registration, accommodation, welcome reception) and close on Thursday, September 23, 1999 around noon.

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

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

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

UMBELLA WORKSHOP on HIGH FREQUENCY EPR, October 21-22, 1999, Nijmegen, The Netherlands.

The UMBELLA project (Ultra High Magnetic fields for Biological EPR) was started in 1996 and supported by the European Community to develop high frequency EPR options as part of the high magnetic field user-facility in Nijmegen. At present the facility provides EPR spectroscopy up to 300 GHz in fields up to 18 Tesla or, if needed, up to 30 Tesla. Potential users from Biology, Chemistry or Physics that are interested to explore

the merits of high frequency EPR are cordially invited to participate in the opening workshop that will be held on october 21 and 22 in Nijmegen, The Netherlands.

The workshop is dedicated to exploring the current possibilities of high frequency high field EPR and to set up international co-operations in this field. Experienced HF-EPR spectroscopists as well as biochemists and physicists from various fields will present their work illuminating the role of HF-EPR in their research. The workshop will also include tutorials on sensitivity and sample handling. (Bio)chemists and material scientists who are interested in using HF-EPR are therefore especially welcome to join this workshop.

Inquiries and further mailings: Contact Dr. E.J. Reijerse; (rey@sci.kun.nl) or Drs. E. van der Horst (ericvdh@sci.kun.nl); Secretary: Mrs. D.D. van der Wey, (desiree@sci.kun.nl); Department of Molecular Spectroscopy, Faculty of Science, Mathematics and Informatics, Toernooiveld 1, 6525 ED Nijmegen. Or, surf to the web page at:

http://www.sci.kun.nl/hfml/hfepr

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

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

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

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

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

http://www.ied.edu.hk/has/phys/apepr/index.htm

XIXth INTERNATIONAL CONFERENCE on MAGNETIC RESONANCE in BIOLOGICAL SYSTEMS (XIX ICMRBS), Florence, Italy, August 20-25, 2000.

You are cordially invited to attend the XIXth International Conference on Magnetic Resonance in Biological Systems (XIX ICMRBS) to be held in Florence, Italy from August 20 to 25, 2000. Florence is easily accessible both by train (ca. 1.5 hrs from Rome by fast train) and by plane. The airport, located 5 Km from the city center, is connected, through direct flights, with the major Italian and European cities.

Scientific Program–The scientific program will cover a wide range of research topics in the field of magnetic resonance applied to biological systems. Particular attention will be devoted to new and promising areas of research as well as to emergent methodological tools within the frame of NMR research in the post-genomic era. The scientific agenda will include plenary lectures, session lectures and poster presentations. The sessions will be organized on the following topics: protein structure, folding, and mobility; EPR/ENDOR applications; membrane proteins; In vivo spectroscopy and imaging; DNA, RNA,

nucleotides and their interaction with proteins; SAR of drugs and drug discovery; computation and dynamics.

Location–The conference will take place at the Centro Internazionale Congressi and Palaffari Firenze located close to the central railway station in the historical and monumental area of Florence.

Accommodation–Accommodation will be arranged in hotels of different categories, mostly within walking distances from the venue (student dorms will be available). Detailed information and reservation forms for accommodation will be included in the second circular.

Information on the scientific program, accommodation, general arrangements, registration forms and instructions for preparation of abstracts are continuously updated in our web site. Please visit it! Registration can be done on line. Abstract and early registration deadline is March 31, 2000. For further information, please contact: XIX ICMRBS Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi, 7, 50121 Florence, Italy; Fax: +39 - 0552757555 (do not omit the 0); E-mail: ICMRBS@lrm.fi.cnr.it. Or visit the web address at:

http://www.lrm.fi.cnr.it/icmrbs.html

Conference Committees: *Organizers:* I. Bertini, (Florence, Italy) Chairperson; L. Banci (Florence, Italy) Ex. Manager; R. Kaptein (Utrecht, The Netherlands); H. Rueterjans (Frankfurt, Germany); G. Valensin (Siena, Italy). *Assistants to the organizers*: R. Del Conte & I.C. Felli (Florence, Italy); Treasurer: P. Turano (Florence, Italy). International Advisory Board: A.S. Arseniev (Moscow, Russia); C.M. Dobson (Oxford, U.K.); S. Forsen (Lund, Sweden); G. Govil (Bombay, India); A.M. Gronenborn (Bethesda, USA); C.W. Hilbers (Nijmegen, The Netherlands); J.S. Hyde (Milwaukee, USA); C. Ho (Pittsburgh, USA); M. Kainosho (Tokyo, Japan); J.F. Lefevre (Strasbourg, France); J.L. Markley (Madison, USA); A. McDermott (New York, USA); K. Möbius (Berlin, Germany); R.S. Norton (Parkville, Australia); S.J. Opella (Philadelphia, USA); M. Rico (Madrid, Spain); J. Seelig(Basel, Switzerland); B.D. Sykes(Edmonton, Canada); W. Tang (Nanjing, China); G. Varani (Cambridge, U.K.); A. Walker (Tucson, USA). *National Organizing Committee*: Coordinator: A. Rosato (Florence, Italy); S. Aime (Torino); R. Basosi (Siena); R. Bazzo (IRBM); F. Conti (Roma); A. Di Nola (Roma); A. Lai (Cagliari); S. Mammi (Padova); B. Maravigila (Roma); C. Marchioro (Glaxo); G. Martini (Firenze); H. Molinari (Verona); V. Pavone (Napoli); A. Perico (CNR, Italy); F. Podo (Ist. Sup. Sanita); A. Rigo (Padova); A.L. Segre (CNR); A. Spisni (Parma); M. Tato' (Pharm.& Upjohn); P.A. Temussi (Napoli); A. Tomasi (Modena); A. Tramontano (IRBM); F. Uggeri (Bracco); L. Zetta (CNR). *Chairperson of Local Organizing Committee:* R. Pierattelli (Florence, Italy).

POSITIONS AVAILABLE & WANTED

TWO OPENINGS FOR PHD LEVEL MAGNETIC RESONANCE SPECTROSCOPISTS AT PRINCETON UNIVERSITY

MAGNETIC RESONANCE SPECTROSCOPIST-PhD Professional Staff Position: Princeton University has an immediate opening for a Ph.D. level magnetic resonance spectroscopist with preferred experience in, e.g., EPR/ENDOR and solid state NMR spectroscopy. Primary duties involve maintenance of related instrumentation (hardware) and associated peripherals, including all spectrometer components, workstations, cryostats, probes, cavities, resonators and plotters; special projects in hardware design, training of new users on basic as well as advanced techniques; scheduling and bookkeeping of multi-user instruments, educating students and faculty in new magnetic resonance methods and instructor for lectures on the theory of instrument operation; drafting of instrumentation proposals. The spectroscopist will fill one of two Professional Staff positions with complementary skills and overlapping instrument responsibilities in a growing NMR/EPR facility (5 NMRs, 2 EPRs, 1 ENDOR). Send resume to: Prof. Charles Dismukes, Operations Committee, Dept. of Chemistry, Princeton University, Princeton, NJ 08544. Princeton University is an Equal Opportunity/Affirmative Action employer.

Pulsed-EPR/ENDOR Spectroscopist - Postdoctoral Research Scientist: Princeton University has an immediate opening for a recent PhD scientist with experience in pulsed EPR spectroscopy and multiple resonance spectroscopy (ENDOR). Primary responsibilities include applications of these methods via collaborative internal projects with chemists and enzymologists in training (undergraduates, graduate students and postdoctoral scientists). An opportunity exists to learn about recent discoveries in a several areas of scientific research within inorganic chemistry, photochemistry, solar energy conversion, metallo-enzymes, biochemistry and photosynthesis via a collaborative approach. Available spectrometers includes Bruker ESP300E and Elexsys585 spectrometers. For examples of the types of problems consult the publications below or view the Internet web page: http://www.princeton.edu/~catalase/ Send

resume to: Prof. Charles Dismukes, Hoyt Laboratory, Dept. of Chemistry, Princeton University, Princeton, NJ 08544.

- W. Ruttinger And G.C. Dismukes, "Synthetic Water Oxidation Catalysts for Artificial Photosynthetic Water Oxidation," Chemical Reviews, 97, 1-24 (1997).
- Sossong, T.J., S.V. Khangulov, R.C. Cavalli, D.R. Soprano, G.C. Dismukes, and D.E. Ash, "Catalysis on Dinuclear Mn(II) Centers: Hydrolytic and Redox Activities of Rat Liver Arginase." (1997). J. Bioinorganic Chemistry, 2, 433-443.
- Zaltsman, L., E. Bruntrager, G. Ananyev, and G.C. Dismukes, "A Quantitative Kinetic Model for Photo-assembly of the Photosynthetic Water Oxidase from its Inorganic Constituents: Requirements for Manganese and Calcium in the Kinetically Resolved Steps."Biochemistry, 36, 8914-8922 (1997).
- Ruettinger, W., C. Campana, and G.C. Dismukes, "Synthesis and Characterization of a Mn4O4L6 Complex with Cubane-like Core Structure: A New Class of Models of the Active Site of the Photosynthesis Water Oxidase." J. Amer. Chem. Soc., 119, 6670-6671 (1997).
- G.M. Ananyev and G.C. Dismukes, "Calcium Induces Binding and Formation of a Spin-coupled Dimanganese (II,II) Center in the apo-Water Oxidation Complex of Photosystem II as Precursor to the Functional Tetra-Mn/Ca Cluster." Biochemistry, 36, 11342-11350 (1997).
- S.V. Khangulov, T.M. Sossong, Jr., D.E. Ash, G.C. Dismukes, "L-arginine Binding to Liver Arginase Requires Proton Transfer to Gateway Residue His141 and Coordination of the Guanidinium Group to the Dimanganese(II,II) Center." Biochemistry, 37: p. 8539-8550 (1998).
- Zheng, M., and Dismukes, G.C. "Resolution Enhancement in ENDOR Spectroscopy by Distant-Dependent Enhanced ENDOR Phase (DEEP) Spectroscopy: Application to Determination of the Solvation Structure Around Paramagnetic Ions in Disordered Solids" J. Physical Chemistry (B), 102, 8306-8313 (1998).
- Dismukes, G.C., Ruettinger,W., Boelrijk, A.E.M., Ho, D., "Structure of the Mn4ca1 Core of the Psii Water Oxidizing Complex and the Mn4o4-cubane/ Mn4o2-butterfly Model Complexes," in Proceedings XIth International Photosynthesis Congress, G. Garob, Editor. 1998, Kluwer Academic: Dordrecht.
- Ananyev, G.M., Zaltsman, L., McInturff, R.A. & Dismukes, G.C. (1998) "Assembly Intermediates and "Inorganic Mutants" of the PSII Oxygen Evolving Complex" in Proceedings XIth International Photosynthesis Congress, G. Garob, Editor. 1998, Kluwer Academic: Dordrecht.
- Khangulov, S.V., V.N. Gladyshev, G.C. Dismukes, and T.C. Stadtman, "Selenium Containing Formate Dehydrogenase H from E. Coli: A Molybdopterin Enzyme that Catalyzes Formate Oxidation without Oxygen Transfer." Biochemistry, 1998. 37: p. 3518-3528.

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

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

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

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

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

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

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

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

POST-DOCTORAL POSITION AVAILABLE at NIEHS

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

POST-DOCTORAL POSITION at LEIDEN UNIVERSITY DEPARTMENT of BIOPHYSICS

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

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

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

POSTDOCTORAL FELLOWSHIP AVAILABLE, NCI/NIH, BETHESDA,MD, USA.

EPR spectroscopist for investigations of the mechanism of the synergistic effects of ultrasound and drugs and of sonochemistry and other areas of current biomedical interest. Less than five years of postdoctoral experience with a Ph.D. in chemistry, biochemistry, or biophysics. The initial appointment is for 2 years, starting at $29,000 (or higher depending on experience) plus medical insurance. Please send curriculum vitae to Peter Riesz, Senior Investigator, Radiation Biology Branch, Building 10, Room B3B69, NIH, Bethesda, MD 20892-1002,USA; ☎: 301-496-4036; Fax: 301-480-2238, E-mail: sono@helix.nih.gov

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EPR SPECTROSCOPIST SEEKING POSITION

EPR spectroscopist seeks academic position. Education: M.Sc.: Molecular Spectroscopy, Kazan State Univ., Kazan, Russia. Ph.D.: EPR of tris-chelate transition metal complexes in the liquid- crystalline matrix, 1987, Kazan Phys.-Tech. Inst., Russ. Acad. Sciences, Kazan, Russia. Research experience: EPR of metal- containing liquid crystals or metallomesogens, EPR of paramagnetic transition metal complexes in a liquid- crystalline matrix, EPR of spin-equilibrium and cluster systems, EPR line shape of orientationally ordered solid systems. Experience in maintenance of EPR spectrometers and their additional equipment, computerized data processing, EPR simulations.

Contact Dr. Natalia Domracheva, Kazan Phys.-Technical Inst, 420029, Sibirsky Trakt 10/7, Kazan, Russia. E-mail: domracheva@sci.kcn.ru.

EQUIPMENT & SUPPLIES EXCHANGE

FOR SALE: BRUKER ESP-300 RADIOSPECTROMETER

For sale: Bruker ESR-300, manufactured and put into operation in 1989. The device is in excellent condition. Bruker's price in 1989 was $510,000. For further information, contact Prof. Roman Eismont, ☎: 7-812-249-02-95; FAX: 7-812-249-51-14; E-mail: empire@peterlink.ru; Regular mail: 6 Shafirovsky Avenue, St. Petersburg 195273 Russia.

AVAILABLE: ISOTOPE-CONTAINING SPIN PROBES

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

WANTED: MICROWAVE BRIDGE

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

FOR SALE - NMR MAGNETOMETER

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

WANTED: USED VARIAN SPECTROMETER

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

WANTED: VARIAN MICROWAVE BRIDGE

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

JEOL TE2000 SPECTROMETER

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

AVAILABLE: VARIAN COMPONENTS and MAINTENANCE

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

http://www.webspace.it/vpnmr

FOR SALE: VARIAN

Resonance Instruments has available:

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

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

NEED HELP in DESIGN and CONSTRUCTION of EPR ELECTRONICS?

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

AVAILABLE: TWO IBM 9000 COMPUTERS

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

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

AVAILABLE: USED VARIAN EPR EQUIPMENT:

1) Two Varian E-3's are in the process of being refurbished. I expect to have them ready in early spring of 1999. They will

meet factory specifications and will come complete with a one year warranty. The units may also include some upgrades.

2) Varian ENDOR accessory, with Varian ENDOR cavity.

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

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

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

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

FOR SALE: VARIAN SYSTEM

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

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

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WANTED: X-BAND BRIDGE

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

IES MEMBERS WHOSE MAIL HAS BEEN RETURNED

Below is a list of members whose mail has been returned to the IERC, along with their last-known country. ***Please contact the IERC if you know the current e-mail and/or address of any of these members:***

Atushi, Hawamura (JAPAN)
Batyuk, V. A. (RUSSIA)
Bigelow, Diana J. (USA)
Bosch, Martin K. (NETHERLANDS)
Buy, Clotilde (FRANCE)
Chen, Guoman (CANADA)
Clardy, Roxanne (USA)
Coan, Carol R. (USA)
Coyne, Lelia M. (USA)
Cybulski, Mariusz (POLAND)
Dijk, B. van (NETHERLANDS)
Gaevoi, Vasil Alexeyevich (UKRAINE)
Garrett, R. W. (AUSTRALIA)
Goldberg, Seth (USA)
Hamburger, Steven A. (USA)
Helle, Norbert (GERMANY)
Holder, Sonya L. (USA)
Ito, Shosuke (JAPAN)
Iyer, Pradeep S. (USA)
Jent, Francisco (SWITZERLAND)
Jung, Paul (BELGIUM)
Kaysser, Tamma M. (USA)
Kobayashi, Tadashi (JAPAN)
Kormanovsky, Alexander Ya. (RUSSIA)
Kozlov, A. V. (RUSSIA)
Larsen, Russell (USA)
Lewellen, Terri (USA)
Long, Stephen M. (USA)
Marov, I. N. (RUSSIA)
Mieghem, Frans Van (FRANCE)
Morris, Andrea (USA)
Nienaber, Vicki L. (USA)
Nyman, Philip D. (USA)
Pedersen, Jens A. (DENMARK)
Polishchuk, V. E. (UKRAINE)
Rashba-Step, Julia (USA)
Rehfeld, Selwyn J. (USA)
Roble, Jim (USA)
Safrazyan, Nina L. (RUSSIA)
Sergeev, A. (RUSSIA)
Shi, Shu (SINGAPORE)
Shiryaeva, Olga A. (RUSSIA)
Slane, Jean M.K. (USA)
Sonoda, Masaru (JAPAN)
Tan, Xiaoling (USA)
Trif, Eleonora (AUSTRALIA)
Vacek, Karel (CZECHOSLOVAKIA)
Vrieze, Jacobien (NETHERLANDS)
Wallner, Peter H. (AUSTRALIA)
Warren, William L. (USA)
Wu, Maoxin (USA)
Yang, George C. (USA)
Zhang, Yong-Kang (USA)
Zimmer, Guido (GERMANY)
Zubarev, Valentin E. (GERMANY)

Bacon, Pamela J. (UK)
Bensebaa, Farid F. (USA)
Bogumil, Ralf (GERMANY)
Brown, Ian P. (USA)
Bystrov, V. F. (RUSSIA)
Chen, Feng (USA)
Cleary, David A. (USA)
Coninckx, Francois (SWITZERLAND)
Crowder, Mark S. (USA)
Dejehet, Fernand G. (BELGIUM)
Fronko, Richard M. (USA)
Gorbatenkova, E. A. (RUSSIA)
He, Wei Z. (USA)
Hirschfelder, Monika (GERMANY)
Iamnova, M. A. (RUSSIA)
Ivancich, Anabella (FRANCE)
Jasty, Shashi (USA)
Jia, Kang Han (PRC)
Kalaw, Benito O. (USA)
Keiichi, Mitsuta (JAPAN)
Kroneck, Pans C. (GERMANY)
Lassmann, Gunter (GERMANY)
Linhares, Marilia P. (BRAZIL)
Lorigan, Gary (USA)
Marshall, S. A. (USA)
Miller, Allen J. (USA)
Narayanaswami, Vasanthy (USA)
Niesman, Michael (USA)
Pavlova, Valentina M. (RUSSIA)
Pelekh, Alexey E. (RUSSIA)
Randall, David W. (USA)
Reczkowski, Robert S. (USA)
Rius, Gerard (FRANCE)
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Secourgeon, Li Liane (FRANCE)
Sharashenidze, Z. A. (REP. GEORGIA)
Shin, Dae-Ho (KOREA)
Sibley, Scott P. (USA)
Snyder, Seth W. (USA)
Sun, Xiao-Ya (USA)
Tommos, Cecilia (SWEDEN)
Tse, Susanna Y. (USA)
Vesnin, Y. I. (RUSSIA)
Wolfrum, Edward J. (USA)
Xu, Ruixin (USA)
Yarema, Kristin A. (USA)
Zhang, Youping (CANADA)
Zou, Yue (USA)

RECEIVED AT PRESS TIME: POSSIBLE MEETING on INDUSTRIAL APPLICATIONS of EPR/ESR

Attention: Are you interested in contributing to and/or attending a meeting tentatively planned for October 1999 in Bloomington, IL on industrial applications of EPR/ESR? If so, please contact Clarence Arnow (rii@wwa.com) or Reef Morse (reef@xenon.che.ilstu.edu).

E-MAIL INFORMATION AVAILABLE ON WEB

Since e-mail has become a popular means of communication, having correct e-mail addresses is vital. The directory issue helps, but we receive changes almost every day. To assist in communications among EPR researchers, we have put our list of e-mail addresses on the IES WWW. It is updated monthly. Please check your own e-mail address on the Web and tell us if your address should be added or corrected. The WWW address:

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.

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EPR NEWSLETTER

Volume 10, Number 2 Page 1 1999-2000

IMPORTANT IES BUSINESS:
Election of New Officers & Proposed Revisions to the IES Constitution (See pp. 18 ff)
PLEASE VOTE

From the Editor

Greetings from Illinois. I write this in the heat of our summer. In the central Midwestern USA, summertime means warm humid air that, even with excellent air conditioning, fogs the air and ices the outlet stacks of the cryostats in our EPR spectrometers. Maybe a reader has a neat trick to share with us in the Tips and Techniques column that will help combat this or any other little vexing problems that plague EPR experimentalists. If so, please contact the editorial office. News of interest to the EPR community, material suitable for a regular article, letter to the editor, conference information, or the like is also welcome.

To all the members of the International EPR Society, please check to see whether you have paid your Society dues for 1999. That information, and instructions for paying your dues, is accessible through a link on the Society's Web site: http://IES.scs.uiuc.edu.

Dues are convenient to pay by credit card or check. *They are modest, being set to just barely cover the cost of production and distribution of the Newsletter, maintenance of the Society databases, and minimal Society business expenses such as those connected with awards presentations. It will help keep the IES dues at a low level and allow the society to maintain and expand services if you could get your EPR-active colleagues and friends to join. It's especially important to encourage the young people to join. There are special inexpensive membership rates for students and postdoctorals.*

Finally, please cast your votes on the proposed revised IES Constitution and new IES officers - see p. 2 and Appendix.

R. Linn Belford, Urbana, Illinois, USA

1999 IES Medalists Announced

✦✦✦✦✦✦✦✦✦✦✦✦✦

GOLD MEDAL:

Prof. Brian Hoffman
(Northwestern University)

SILVER MEDALS:

Silver Medal in Biology/Medicine:
Prof. Jack Peisach
(Albert Einstein College of Medicine)

Silver Medal in Physics/Instrumentation:
No 1999 award

Silver Medal in Physics/Materials Science:
Prof. George Watkins
(Lehigh University)

Silver Medal in Chemistry:
Prof. Yuri Tsvetkov
(Institute of Chemical Kinetics/Combustion, Novosibirsk)

YOUNG INVESTIGATOR:

Ilya A. Shkrob
(Argonne National Laboratory)

IES FELLOWS:

Melvin P. Klein (University of California, Berkeley)
Martyn Symons (University of Essex)
Hans Christoph Wolf (University of Stuttgart)

✦✦✦✦✦✦✦✦✦✦✦✦✦

Full written citations for all 1999 IES award winners will appear in a future edition of the *EPR Newsletter.*

•Newsletter Editor: R. Linn Belford, Urbana, IL
•Assistant Editor, Becky Gallivan, Urbana, IL
•Typography: Martha Moore, Urbana, IL.
*•This, the official newsletter of the **International EPR(ESR) Society**, is supported by the Society, by corporate and other donors, and by the National Center for Research Resources in the U.S. National Institutes of Health. For additional information including how to contact the editor, see "About This Publication" on p. 17.*

IN THIS ISSUE

EPR NEWSLETTER Volume 10, Number 2
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✦ IES AFFAIRS ✦

ANNOUNCEMENTS AND REPORTS FROM THE INTERNATIONAL EPR (ESR) SOCIETY

From the Secretary —

Toward a new Constitution: During my time as Secretary of the Society, it has became apparent that there were several aspects of the Constitution under which we are meant to operate which no longer worked. I have sought therefore to rewrite the Constitution in the hope that we will have a document that will work well for the Society for the foreseeable future and make the task easier for all Office Bearers. The Appendix to this Newsletter contains a draft of the proposed new Constitution together with an expanded discussion of the changes and arguments for them. A ballot is attached. Please use this ballot to cast your vote.

New Officers: Please vote for new IES officers. Use the ballot in the Appendix to this Newsletter.

John Pilbrow
Secretary, International EPR Society

IES Awards —

Previous IES Awards Winners

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

Arnold Hoff Wins 1999 Voevodsky Prize

✦✦✦✦✦✦✦✦✦

We are pleased to announce that the Voevodsky Prize Committee has selected Prof. Arnold Hoff (Leiden University) as the 1999 Voevodsky Prize winner. Prof. Hoff was selected for his outstanding contributions to the investigation of primary photochemical and photophysical processes in photosynthetic energy conversion by using radiospectroscopy method. A profile of Prof. Hoff will appear in a future issue of the *EPR Newsletter*.

Yuri D. Tsvetkov
Russian Academy of Sciences, Novosibirsk

1999 Zavoisky Prize to Joan van der Waals

✦✦✦✦✦✦✦✦✦

Following extensive nominations from the international community of EPR scientists, the International Zavoisky Award Committee is delighted to announce that the Zavoisky Awardee for 1999 is Professor Dr. Joan van der Waals (Leiden). He will be awarded the Prize at the annual Workshop "Modern Development of Magnetic Resonance," to be held in Kazan 21-25 September 1999. Prof. J. van der Waals is distinguished for the laureate's work in electron paramagnetic resonance and, in particular, his outstanding contributions to the investigation of photo-excited triplet state molecules. A further citation of his work will appear in a forthcoming issue of *Applied Magnetic Resonance*.

Professor Kev Salikhov
Chairman of the Zavoisky Award Committee

1999 Bruker Prize to Jan Schmidt

✦✦✦✦✦✦✦✦✦

The 1999 Bruker Prize has been awarded to Prof. Jan Schmidt of the University of Leiden, Netherlands. A full profile of Prof. Schmidt will appear in a future edition of the *EPR Newsletter*.

Deadlines Set for Newsletter Materials —

Henceforth there will be firm and fast deadlines for the receipt of materials for each issue of the *EPR Newsletter*. They will be published in each issue of the newsletter and on the *EPR Newsletter* web page, and the next deadline is:

Volume 10 Number 4: **November 8, 1999.**

EPR SPECIALIST VIGNETTES

Edited by
Arthur Schweiger

EPR Study of Atoms Encapsulated in Fullerenes

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Introduction

Performing spectroscopy of particles in traps always was an attractive goal for physicists and chemists. Two features of traps contribute to this attractiveness: First, otherwise elusive particles can be stabilized, and second, the interaction of a particle with its surrounding can be minimized thus enabling the study of its intrinsic properties. Since the discovery of Fullerenes with their appealing 3-dimensional structure it was obvious that atoms or ions could in principle be encased by these all-carbon molecules. In the meantime, a significant number of elements of the periodic table has been encapsulated in Fullerenes. Initially, group III elements like Scandium, Yttrium, and Lanthanum were encapsulated during the Fullerene synthesis by a hitherto unidentified process. Pioneering work of the IBM group at SanJosé[1] and researchers from Nagoya[2] showed that a characteristic feature of these molecules is first, significant charge transfer from the encased atom to the carbon shell, and second, localization of the ion at specific positions at the inside of the carbon cage, i.e., the formation of a mixed ionic/covalent bond. For this reason, these components, whose presence could be detected in trace quantities because of their paramagnetism, must rather be described as "internal salts" and therefore did not qualify as "chemical traps."

This particular feature was first realized, when Saunders succeeded in incorporating Helium atoms in C_{60} by applying pressure and elevated temperatures.[3] Although only up to 10^{-3} "cages" were filled using this procedure, the capability of NMR for a selective detection of ^{3}He isotopes gave clear evidence that stable gases can be encapsulated in Fullerenes. As anticipated, different cages (C_{60}, C_{70}, and Fullerenes chemically modified by addition reactions) could be identified by characteristic differences in their chemical shift values.[4]

Compared with both rather crude preparation techniques, encapsulation by molecule/atom (ion) collision has the advantage that the "synthesis" mechanism can be studied in detail, in particular the energy dependence of the reaction cross section can be compared with predictions from Molecular Dynamics calculations. Early experiments by Schwarz [5] showed that optimal collision energies are in the range of 20 - 40 eV, large enough to allow penetration and not too high to allow for reformation of the temporarily disrupted carbon cage.

The idea of ion bombardment for atom encapsulation was used by Weidinger[6] and also by Campbell[7] for a production of macroscopic quantities of encased atoms. In the group of Campbell, alkali ions (in particular Lithium) were used. Mass spectroscopy and IR as well as Raman experiments gave evidence for the existence of stable Li@C_{60}. Unfortunately, no EPR signals of the paramagnetic species of group I elements could be detected, although solutions of HPLC-separated probes were investigated. Most likely, dimerization leads to the formation of diamagnetic products thus preventing unambiguous identification by EPR via the characteristic hyperfine interaction with the various magnetic isotopes of the alkali metals.

In contrast, group V elements like Nitrogen and Phosphorus, which were also incorporated by ion bombardment in the group of Weidinger, could be characterized and identified by EPR, giving clear proof of the, quartet spin ground state of the encapsulated neutral atom.[6, 8-10] These compounds show vanishing electron and/or spin transfer to the carbon shell and – in this respect – behave like the noble gas/Fullerene systems. Because of their inherent paramagnetism, even trace quantities can be studied.

In this contribution, earlier results of NMR studies of noble gases in Fullerenes are first briefly reviewed. Then a compilation of EPR studies of Group III elements is given. Finally, I describe more recent results obtained for the group V elements, which can be envisaged as prototypes of atoms in

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chemical traps and which can be studied with high sensitivity by EPR.

1. Noble gases inside Fullerenes

After having shown by thermal release experiments that noble gases, in particular Helium, can be trapped in minute quantities in C_{60} under the conditions of standard synthesis of Fullerenes by arc burning of graphite rods in a Helium atmosphere, the combination of elevated temperatures (920 K) and moderate pressure ($3 \cdot 10^8$ Pa) was found to yield bulk quantities of Fullerenes with He atoms incorporated at a surprisingly high level. Using C_{60} and C_{70} for trapping, all noble gases could be encased up to the 10^{-3} level (with the exception of a somewhat lower value for Xenon).

With ^{3}He as probe, the capability of Fullerenes to shield external magnetic fields was tested. First experiments with C_{60} and C_{70} gave chemical shifts of −6.4 ppm and −28.8 ppm, respectively, and as was found later, these values apparently define the range of values seen for higher Fullerenes and their various topoisomers.[11] Clearly, the single line NMR spectra of $^3He@C_{2n}$, which result from the absence of other magnetic nuclei and/or a vanishing coupling with the ^{13}C nuclei of the cage, can be used as "fingerprint" for the detection of topoisomers from a single mass Fullerene sample. Furthermore, it was also observed that distinct shift values can be attributed to different 6,6-adducts of C_{60} and C_{70}. As expected, chemical shielding is also sensitive to the total charge on the Fullerene cage, as has been demonstrated recently.[12]

Using ^{3}He "labeled" Fullerenes as starting material, chemical reactions involving derivatization can be followed. In addition, these new compounds can be used as tracer materials if high-sensitivity mass spectroscopy in combination with controlled thermal release is used. More recently, Saunders and coworkers succeeded in encapsulating two atoms of Helium in C_{70} [13] and there is also evidence from mass spectroscopy that a stable molecule (N_2) could be encapsulated in C_{70} for the first time.[14]

2. Metallofullerenes (MEF)

This group is characterized by significant charge transfer from the encased atom to the Fullerene cage. Group III derived molecules were most intensively studied because of the relative ease of their production by standard DC arc-discharge methods with metal/graphite composite rods as positive electrodes. In particular, Sc, Y, and La encased in C_{82} could be produced in macroscopic quantities as "HPLC-pure" substances.[15] By using synchrotron X-ray diffraction, not only their "endohedral" nature could be verified but also the predicted off-center position of the metal ion could be confirmed.[16] This topology is in accord with theoretical predictions of strong electron transfer interaction.

Even in the initial stage of crude sample preparation, the MEF could be identified via their characteristic EPR spectra originating from the (isotropic) hyperfine interaction (hfi) of an effective S = ½ electronic spin with the nuclear moment of the metal ion. Well resolved EPR spectra with exceptional narrow lines (5μT typically) were recorded at room temperature in solution, thus rendering these systems ideal candidates for an investigation with pulsed EPR techniques.[17] These experiments could only be interpreted by assuming that first, the ions are rigidly attached to the inside surface of the Fullerenes, and second, that the rotational correlation time of the cage is close to the "free rotator limit" even in solution.[18] Apparently, the unstructured "carbon only" surface of the Fullerenes cannot participate in angular momentum exchange by collisions with solvent molecules. As a result, rotational correlation times in order of 10 ps are observed in low-viscosity solvents, much shorter than values predicted using the standard Stokes/Einstein relation.

Whereas standard c.w. EPR techniques could be used to unravel most of the relaxation processes by analyzing the dependence of the EPR line width on the nuclear spin quantum number m_I of the fully resolved EPR spectrum, 2D EPR had to be invoked to unambiguously identify nuclear quadrupole interaction as dominant mechanism for nuclear spin flips.[17]

Although a lot of detailed studies have been performed in the last years, the situation is less clear than in the case of encased noble gases discussed above. This may result from the fact that group III elements and more recently group II elements can only be encased in higher Fullerenes lacking the high icosahedral symmetry of C_{60} which can exist in a variety of topoisomers.

Apparently, different topoisomers of a Fullerene of specific mass lead to a characteristic hfi with the metal ion, but up to now it is not possible to relate these coupling constants to specific cage topologies. In the case of diamagnetic compounds, 2D ^{13}C NMR can be used for an experimental determination of the cage structure, but because synthesis and purification of a sufficient amount of material is a very challenging task, only very limited information is available. For this reason even the basic question which cage structure nature uses for the most abundant MEF, cannot be answered with certainty.

Recent research on MEF focuses on following questions

1) Is it possible to influence chemical modification of the Fullerene cage by the presence of encased ions?
2) What is the dominant decay mechanism of MEF?
3) Can electronic properties of the metal ions be modified in a predictable fashion?
4) Modeling of charge transfer and binding mechanism with quantum chemical methods.

In most cases EPR can be used as sensitive tool to discriminate between different hypotheses. In particular, an unambiguous method for the determination of spin multiplicities is important for a description of the strongly coupled spin systems of charged Fullerenes and encapsulated ions.

A major break-through in synthesis methods was reached when Weidinger's group (HMI, Berlin) [6] and Campbell's group (Max Born Institut, Berlin) [7] used ion bombardment for a selective generation of Endofullerenes. In the context of MEF, the results of Campbell and coworkers are briefly reviewed. In their approach, alkali ions of controlled energy were used for a bombardment of thin Fullerene films. Amazingly large production yields of up to 30% were reported, measured by an analysis of mass spectra. Using HPLC, mass pure MEF were prepared, which could be studied with EPR. Unfortunately, all samples measured so far were found EPR silent in liquid and also in frozen solution at Helium

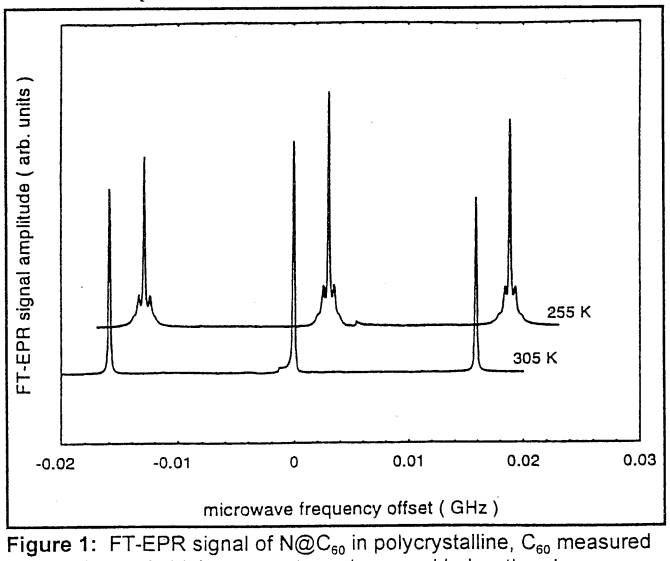

Figure 1: FT-EPR signal of $N@C_{60}$ in polycrystalline, C_{60} measured in the isotropic high temperature phase and below the phase transition to the ordered phase. The additional structure originates from ZFS of the Nitrogen quartet spin located at sites with S_6 symmetry.

temperatures. From this we have to conclude that $Li@C_{60}$ (which was studied most intensively) does not exist as isolated monomer in solution, the absence of an EPR signal being tentatively attributed to dimerization. Final proof of this structure model has to be obtained by NMR experiments.

Localization of the encased ion on the time scale of the EPR experiment (i.e., 1μs) even at room temperature is in accord with quantum chemical calculations providing an estimate for the 3-dimensional potential.[19] The situation changes completely when more than one ion is encapsulated. EPR experiments performed on $Sc_3@C_{82}$ gave compelling evidence for rapid reorientation of the ion trimer within the cage.[20] Values for the reorientational barrier (E = 28 meV) and for the room temperature correlation time (τ (300 K) $\approx 3 \cdot 10^{-9}$ s) were deduced from an analysis of EPR line width data.

Further evidence for internal dynamics was obtained from an NMR study of diamagnetic $Sc_2@C_{84}$.[21] Two different topoisomers were separated and ^{45}Sc NMR spectra were recorded. Much larger activation energies as compared to $Sc_3@C_{82}$ ($\Delta E \approx 0.1$ eV) were deduced from a line shape analysis leading to significantly larger correlation times for the internal relocation processes (τ (300 K) $\approx$ 100 ms) in both topoisomers.

Complete modeling of the internal dynamics of MEF is a formidable task for quantum chemistry. Molecular Dynamics (MD) simulations based on the Car-Parinello approximation successfully predicted localization of the metal ion at specific binding sites.[19] However, these results, which were obtained for a specific topoisomer of C_{82} (that is most probably not corresponding to the cage forming the prominent species), are covering only a time interval of a few ps. Therefore results from EPR and NMR, probing much slower processes, are still out of the range of quantitative predictions.

3. Nitrogen and Phosphorus in Fullerenes

As in the case of Metallofullerenes, EPR could be used to provide evidence for the electronic structure of these new compounds. Nitrogen ENDOR spectra gave proof of the quartet electronic spin state, consistent only with the assumption that neutral Nitrogen atoms are encased and that negligible spin and charge transfer exists to the carbon cage. The "high spin" state of the central atom in turn provides a sensitive tool to test the symmetry of the local potential via Zero-Field-Splitting (ZFS) interaction. Clearly, this term vanishes for an undisturbed isolated C_{60}, but incorporation either in solids with low site

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symmetry or in liquids with collision-induced deformation of the cage will lead to observable effects.

The eigenvalues of a quartet spin system can be completely described by second-rank tensor operators, and the restrictions for observables resulting from the local symmetry at the Nitrogen site are well known. As an example for the applicability of $N@C_{60}$ as local symmetry probe we studied the first-order phase transition of crystalline C_{60} at 256 K. Here, the site symmetry is lowered from T_h to S_6, allowing for the existence of a ZFS of axial symmetry in the low temperature $Pa\bar{3}$ phase. Fig. 1 shows the EPR spectrum of $N@C_{60}$ in polycrystalline C_{60} in the high temperature $Fm\bar{3}m$ and in the ordered $Pa\bar{3}$ phase. The additional lines can be fitted by invoking a ZFS with D = 0.52 MHz. This proved the existence of long range order, although the cages still undergo quasi isotropic reorientation with a correlation time of a few nanoseconds.

Instead of lowering the site symmetry via a crystal field, the cage can also be distorted permanently by addition reactions. In case of $N@C_{61}(COOEt_2)_2$ (**1**), this leads to a ZFS of 8 MHz.[22] From an analysis of spin relaxation times of $N@C_{60}$ in solution, the variance of the collision-induced fluctuating ZFS was determined as 5 MHz,[8] close to the value found for the permanently distorted (Fig. 1). The correlation time τ_c for this fluctuating interaction was approximately 10 ps, a value consistent with the translational correlation time of the solvent molecules. Probing the frequency dependence of T_1 at X and W band, this short value for τ_c could be confirmed. Fig. 2 shows saturation recovery curves for $N@C_{60}$ in CS_2 at room temperature. Whereas T_2 is nearly frequency independent, T_1 increases by a factor of four at the higher Larmor frequency.

A higher "sensitivity" for cage distortions was expected if the larger phosphorus atom is encapsulated. Indeed, a factor-of-10 increase in the collision-induced ZFS was measured.[10] Because of the large isotropic hfi of ^{31}P (a = 147 MHz), second-order hfi splitting of 0.5 MHz made it possible to record the allowed (3/2, 1/2), (1/2, −1/2), and (−1/2, −3/2) EPR transitions separately in a standard c.w. experiment, because the homogeneous line widths at room temperature was only 300 kHz. A full analysis of the spin relaxation mechanisms was possible for the first time for a quartet spin in solution. The values deduced for the temperature dependence at the correlation time confirmed modulation of ZFS by collisions as dominant relaxation process.

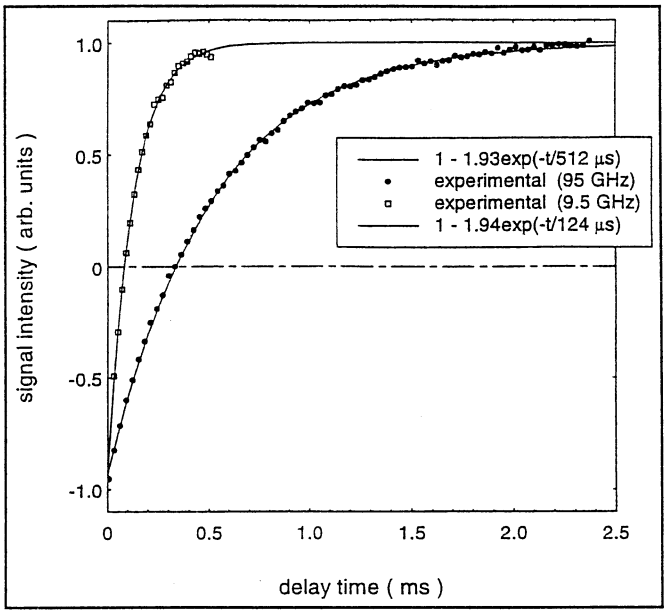

Figure 2: Saturation recovery signals of $N@C_{60}$ in CS_2 at room temperature. The data could be fitted assuming mono-exponential relaxation of the selectively inverted hyperfine component.

4. Outlook

Magnetic resonance techniques have played a major role in unraveling the properties of Endofullerenes. Any attempt to assess the broader applicability of these new compounds has to take into account the stability of the compounds.

Apparently, all species with vanishing charge and spin transfer from the encapsulated atom to the carbon case are superior in this respect. As a result, the diamagnetic noble gas systems as well as the Fullerenes containing the paramagnetic group V elements are most promising. For both classes of molecules it has been established that they are stable on a time scale of years under ambient conditions. Using ^3He as encapsulated atom, straightforward 1D NMR can be used to unravel pathways of multiple chemical reactions, because every product has its own characteristic chemical shift. Apart from possible applications more tedious ^{13}C 2D NMR is necessary to determine the "tertiary structure" of the carbon network forming the cage of group II elements. Here one is still awaiting a consistent picture referring to the realization of trapping cages of a specific mass isomer compared to those realized by nature for "empty" Fullerenes.

The paramagnetic compounds derived from N and P, will probably find their use as probes for changes of local fields resulting for instance by phase transitions in solids or by ordering

transitions in liquid crystals. Additionally, apart from permanent changes of local symmetry, also fluctuating fields originating from paramagnetic centers can be detected by an analysis of the spin relaxation processes. In all these examples one makes use of the high sensitivity of the quartet electron spin state towards deviations of the local charge distribution from cubic symmetry.

Acknowledgement

Collaborations with B. Pietzak, M. Waiblinger, and A. Weidinger (HMI Berlin) as well as with E. Dietel and A. Hirsch (University Erlangen) are gratefully acknowledged. Support from the BMBF (13N6674/5) and DFG (Di 182/19-1) was essential for the success of the investigations.

References

1. R. D. Johnson, M. S. de Vries, J. Salem, D. S. Bethune, and C. S. Yannoni, Nature 355 (1992) 239.
2. H. Shinohara, H. Sato, M. Ohkohchi, Y. Ando, T. Kodama, T. Shida, T. Kato, and Y. Saito, Nature 357 (1992) 52.
3. M. Saunders, H. A. Jimenez-Vazquez, R. J. Cross, and, R. J. Poreda, Science 259 (1993) 1428.
4. R. J. Cross, H. A. Jimenez-Vazquez, Q. Lu, M. Saunders, D. I. Schuster, S. R. Wilson, and H. Zhao, J. Am. Chem. Soc. 118 (1996) 11454.
5. T. Weiske, D. K. Böhme, J. Hrusak, W. Krätschmer, and H. Schwarz, Angew. Chem. Int. Ed. Engl. 30 (1991) 884.
6. T. Almeida Murphy, T. Pawlik, A. Weidinger, M. Höhne, R. Alcala, and J.-M. Spaeth, Phys. Rev. Lett. 77 (1996) 1075.
7. R. Tellgmann, N. Krawez, S.-H. Lin, I. V. Hertel, and E. E. B. Campbell, Nature 382 (1996) 407.
8. C. Knapp, K.-P. Dinse, B. Pietzak, M. Waiblinger, and A. Weidinger, Chem. Phys. Lett. 272 (1997) 433.
9. C. Knapp, N. Weiden, and K.-P. Dinse, Appl. Phys. A 66 (1998) 249.
10. C. Knapp, N. Weiden, H. Käß, K.-P. Dinse, B. Pietzak, M. Waiblinger, and A. Weidinger, Mol. Phys. 95 (1998) 999.
11. M. Saunders, R. J. Cross, H. A. Jimenez-Vazquez, R. Shimshi, and A. Khong, Science 271 (1996) 1693.
12. E. Shabtai, A. Weitz, R. C. Haddon, R. E. Hoffman, M. Rabinovitz, A. Khong, R. J. Cross, M. Saunders, P.-C. Cheng, and L. T. Scott, J. Am. Chem. Soc. 120 (1998) 6389.
13. A. Khong, H. A. Jimenez-Vazquez, M. Saunders, R. J. Cross, J. Laskin, T. Peres, C. Lifshitz, R. Strongin, and A. B. Smith III, J. Am. Chem. Soc. 120 (1998) 6380.
14. R. J. Cross, M. Saunders, and A. Khong, Proc. ECS meeting San Diego (May 1998).
15. H. Shinohara, M. Inakuma, N. Hayashi, H. Sato, T. Kato, and S. Bandow, J. Phys. Chem. 98 (1994) 8597.
16. M Takata, B. Umeda, E. Nishibori, M. Sakata, Y. Saito, M. Ohno, and H. Shinohara, Nature 377 (1995) 46.
17. M. Rübsam, M. Plüschau, P. Schweitzer, K.-P. Dinse, D. Fuchs, H. Rietschel, R. H. Michel, M. Benz, and M. M. Kappes, Chem. Phys. Lett. 240 (1995) 615.
18. M. Rübsam, P. Schweitzer, and K.-P. Dinse, J. Phys. Chem. 100 (1996) 19310.
19. W. Andreoni and A. Curioni, Phys. Rev. Lett. 77 (1996) 834.
20. P. H. M. van Loosdrecht, R. D. Johnson, M. S. de Vries, C.-H. Kiang, D. S. Bethune, H. C. Dorn, P. Burbank, and S. Stevenson, Phys. Rev. Lett. 73 (1994) 3415.
21. Y. Miyake, S. Suzuki, Y. Kojima, K. Kikuchi, K. Kobayashi, S. Nagase, M. Kainosho, and Y. Achiba, J. Phys. Chem. 100 (1996) 9579.
22. B. Pietzak, M. Waiblinger, T. Almeida Murphy, A. Weidinger, M. Höhne, M. Höhne, E. Dietel, and A. Hirsch, Chem. Phys. Lett. 279 (1997) 259.

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2ND INTERNATIONAL INTERCOMPARISON on EPR TOOTH DOSIMETRY

After nuclear and radiation accidents, the problem arises of determining the amount of ionizing radiation people have been exposed to. This is usually done retrospectively, with environmental dosimetry and modeling, which are valid techniques for estimating the exposure of groups of population. Unfortunately, they are not capable to evaluate individual doses so that cases of persons who were individually exposed to unexpected high doses can not be put in evidence. Retrospective determination of exposure of individuals to ionizing radiation can be performed with methods able to measure the damage induced by the ionizing radiation on biological tissues. Among the several biological methods proposed in the last years, Electron Paramagnetic Resonance of tooth enamel is one of the most reliable. Many biological tissues have been taken under consideration to this purpose in the past, but the bone-like tissues, and in particular the tooth enamel, have turned out to be the best in terms of reproducibility, sensitivity and time stability. The method is based on the measurement of the CO_2^- radical concentration induced by ionizing radiation in the inorganic hydroxyapatite matrix. The most frequently asked question is about the way the teeth are collected. Since it would be too invasive to extract a tooth for dosimetric purposes, measurements are performed with teeth extracted for other reasons, that are, most frequently, deciduous, wisdom and elder people teeth.

In 1996, the European Commission (EC) approved the project "Dose Reconstruction" in the framework of the Nuclear Fission Safety programme (Fourth Framework Programme). The project was aimed to the development, standardization and application of methods for retrospective determination of exposure to ionizing radiation following nuclear accidents. Tooth dosimetry with EPR was one of the methods included in the project. The aim, as far as concerns tooth enamel/EPR dosimetry, was to determine the validity and reliability of the technique, since until then only promising results had been published. GSF (Neuerburg, Germany), as the coordinating Institute, and ISS (Rome, Italy) were the official partners of the EPR sub-project. Utah University (USA) was invited to participate and various Institutes of the former Soviet Union (RPI, Kiev, Ukraine; IMP, Ekaterinburg, Russia; MRRC, Obninsk, Russia) joined the collaboration in the framework of the EC "INCO-COPERNICUS" projects "Dose Reconstruction for Workers of Mayak and for Techa Riverside Residents" and "Dose Reconstruction for Populations in Areas Contaminated by Chernobyl Fallout". At the end of the project, each participant Institute had to deliver a protocol for EPR dose assessment using tooth enamel. The protocols are structured in three sections: tooth enamel sample preparation, CO_2^- signal intensity

evaluation and dose estimate. At the end of the project, there was a call for an International Intercomparison, organized by the project partners, with assistance of the IAEA (Vienna, Austria), open worldwide. The Intercomparison was designed to demonstrate the present state of the art of the tooth enamel/EPR dosimetry in the (0.1÷1) Gy dose range. Twenty participants from all over the world applied. Each participant was asked to provide 5 molars (MRRC provided teeth for those participants who were not in the position to collect teeth). All teeth were irradiated to unknown doses by IAEA with a ^{60}Co source in a PMMA phantom. For each participant, 4 teeth were irradiated in the range 0-500 mGy and one in the range 500-1000 mGy. The results were collected by the IAEA and discussed during the contractors meeting of the "Dose Reconstruction" project held at ISS, Rome, May 6-7, 1999. The results of the Intercomparison will be presented at the LED99 Conference in Rome, September 6-10, 1999.

The collaboration group includes S. Onori, D.Aragno, P.Fattibene of the Istituto Superiori di Sanità (Rome, Italy) and A. Wieser of the Institüt für Strahlenschutz (Neuherberg, Germany). A web site for the collaboration group will be accessible by late summer of 1999.

For further information contact Paola Fattibene, Istituto Superiore di Sanità, Physics Laboratory, Viale Regina Elena 299, I-00161 Rome, Italy; ☎: 39-06-4990-2466; FAX: 39-06-4938-7075; E-mail: Paola.Fattibene@iss.it.

Submitted on behalf of the partners of the European Union projects (Dose Reconstruction; Dose Reconstruction for Workers of Mayak and for Techa Riverside Residents; Dose Reconstruction for Populations in Areas Contaminated by Chernobyl Fallout).

Building the Perfect Beast

by Chris Bender
bender@spin.aecom.yu.edu

SPIN DENSITY DISTRIBUTIONS and VOLUME INTEGRALS

At a Gordon Conference poster session I encountered a presentation by an organic chemist who was using *ab initio* SCF methods (GAUSSIAN) to predict electronic structure and the associated spin density of various organic radicals. What I found somewhat unusual about his poster was the manner in which he displayed the spin density distribution. You often find papers in which the user of an *ab initio* program displays an electronic charge distribution as lobes or three-dimension contour plots about a skeleton that is represented by the nuclear coordinates. The author of this poster did something similar with spin density. He was happily handing out illustrations of his presentation, and the accompanying figure is a reproduction of one of his spin density distribution plots.

These spin density diagrams are generated by a program written by the author of the poster, and my guess would be that this code operates in the same manner as the routines in GAUSSIAN or GAUSSView that generate electron density

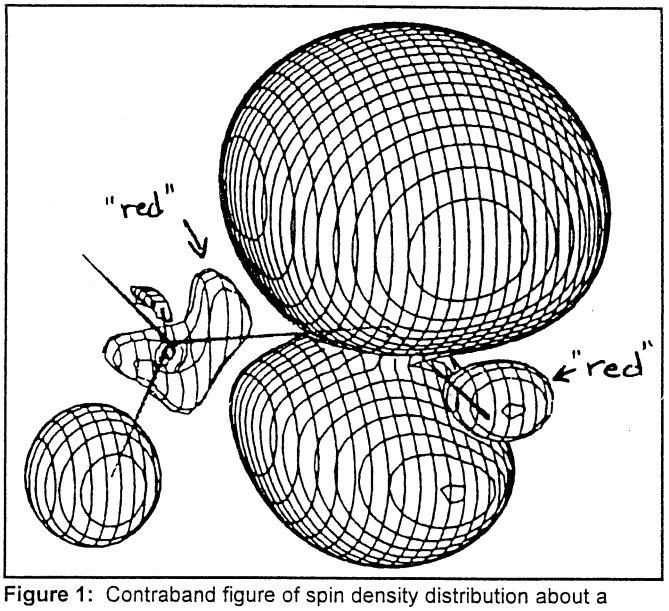

Figure 1: Contraband figure of spin density distribution about a open-shell molecule as derived from the output of an *ab initio* MO calculation.

distribution. In other words, you take the coefficients of the Slater determinant (i.e. the density matrix) and assign a charge based on the spatial coordinate and expectation value (square of the coefficients for the basis function – see Szabo & Ostlund, 1996). For a spin density distribution, one could do the same thing except that alpha and beta spin functionals would be registered, and the "spin density" represented by the difference of the alpha and beta populations.

We are accustomed to analyzing hyperfine spectra by the McConnell relation: $A = Q\rho$, where the terms Q and ρ are the McConnell constant and spin density, respectively. Q has its origin in the perturbational analysis of state admixture that leads to the Fermi Contact interaction involving π-orbitals, which, because of the node at the nuclear center, cannot rigorously possess a Fermi Contact interaction. Q can be derived by using MO theory, but more often than not is an empirical parameter that is constant for a given class of hyperfine interaction (e.g. α-protons, β-protons, etc.).

For protons, Q is usually a single constant value, but for the hyperfine interaction between non-spherical atoms (e.g. ^{13}C and ^{14}N) the hyperfine interaction is expanded into a series $A = \sum Q_i\rho_i$ where the subscript i denotes individual molecular orbitals that possess unpaired spin density character. In other words, for trigonal >N- with sp^2 hybridized orbitals, one would

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write an expansion for each of the sp^2 orbitals and the remaining p-orbital.

The connection to the ab initio spin density distribution is therefore this: an integral is nothing more than an infinitesimal sum of a spatial function in two or more dimensions (area under a curve or volume enclosed by a surface), and one could imagine that the spin density distribution that is represented in the figure might be modified so that it becomes analogous to the McConnell expansion, in other words, $A = \int Q\rho d\tau$, using the usual surface integral terminology. Knowledge of the Q functional would be difficult to maintain, but an equally interesting question arises if one realizes that A is an experimentally measured quantity and ρ is obtained from the electronic structure calculations – one speculates as to whether an integral transform might be used to determine the functional Q.

References:

Szabo, A.; Ostlund, N.S. (1996) Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, New York.

GAUSSIAN and GAUSSView are SCF program packages for MO calculations; both are available from GAUSSIAN Inc., Pittsburgh, PA (http://www.gaussian.com/).

Books and Proceedings

Present and Future of HF EPR Instrumentation

Proceedings published in Journal of Magnetic Resonance

In March, 1998, the Illinois EPR Research Center held a Workshop in Urbana, Illinois entitled "International Experts' Workshop on the Present and Future of HF EPR Instrumentation." It was planned to encourage intensive discussion among the 50 participants, and finished with a wrap-up round-table discussion moderated by Gareth Eaton. Attendees were invited to submit manuscripts for review and publication together in an issue of the Journal of Magnetic Resonance. That issue, Volume 16, Number 2, 1999 is now available and contains the following articles:

NOTICES of MEETINGS

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

UMBELLA WORKSHOP on HIGH FREQUENCY EPR, October 21-22, 1999, Nijmegen, The Netherlands.

The UMBELLA project (Ultra High Magnetic fields for Biological EPR) was started in 1996 and supported by the European Community to develop high frequency EPR options as part of the high magnetic field user-facility in Nijmegen. At present the facility provides EPR spectroscopy up to 300 GHz in fields up to 18 Tesla or, if needed, up to 30 Tesla. Potential users from Biology, Chemistry or Physics that are interested to explore the merits of high frequency EPR are cordially invited to participate in the opening workshop that will be held on October 21 and 22 in Nijmegen, The Netherlands.

The workshop is dedicated to exploring the current possibilities of high frequency, high field EPR and to set up international co-operations in this field. Experienced HF-EPR spectroscopists as well as biochemists and physicists from various fields will present their work illuminating the role of HF-EPR in their research. The workshop will also include tutorials on sensitivity and sample handling. (Bio)chemists and material scientists who are interested in using HF-EPR are therefore especially welcome to join this workshop.

Inquiries and further mailings: Contact Dr. E.J. Reijerse; (rey@sci.kun.nl) or Drs. E. van der Horst (ericvdh@sci.kun.nl); Secretary: Mrs. D.D. van der Wey, (desiree@sci.kun.nl); Department of Molecular Spectroscopy, Faculty of Science, Mathematics and Informatics, Toernooiveld 1, 6525 ED Nijmegen. Or, surf to the web page at:

http://www.sci.kun.nl/hfml/hfepr

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

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

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

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

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

http://www.ied.edu.hk/has/phys/apepr/index.htm

HIGH-FREQUENCY ELECTRON PARAMAGNETIC RESONANCE: TECHNOLOGY AND APPLICATIONS, Amsterdam, The Netherlands, April 12-14, 2000

This conference is being organized under the auspices of the Academy Committee for Chemistry of the Royal Netherlands Academy of Arts and Sciences. The local organizing committee consists of Peter Gast, Edgar Groenen, Arnold Hoff, and Jan Schmidt. The aim of the conference is to report on the progress in the technology of High-Frequency EPR and on applications in physics, chemistry and biology. The program will consist of invited and contributed lectures and poster presentations. A brochure accompanies this newsletter. Scientists interested in contributing to or participating in this conference are invited to contact the web page:

http://www.knaw.nl/hfepr

For further information contact Mr. R. des Bouvrie, Royal Netherlands Academy of Arts and Sciences, P.O. Box 19121, 1000 GC Amsterdam, The Netherlands; E-mail: roy.des.bouvrie@bureau.knaw.nl; ☎: 31-20-55-10-730; FAX: 31-20-62-04-941.

XIXth INTERNATIONAL CONFERENCE on MAGNETIC RESONANCE in BIOLOGICAL SYSTEMS (XIX ICMRBS), Florence, Italy, August 20-25, 2000.

You are cordially invited to attend the XIXth International Conference on Magnetic Resonance in Biological Systems (XIX ICMRBS) to be held in Florence, Italy from August 20 to 25, 2000. Florence is easily accessible both by train (ca. 1.5 hrs from Rome by fast train) and by plane. The airport, located 5 Km from the city center, is connected, through direct flights, with the major Italian and European cities.

Scientific Program–The scientific program will cover a wide range of research topics in the field of magnetic resonance applied to biological systems. Particular attention will be devoted to new and promising areas of research as well as to emergent methodological tools within the frame of NMR research in the post-genomic era. The scientific agenda will include plenary lectures, session lectures and poster presentations. The sessions will be organized on the following topics: protein structure, folding, and mobility; EPR/ENDOR applications; membrane proteins; In vivo spectroscopy and imaging; DNA, RNA, nucleotides and their interaction with proteins; SAR of drugs and drug discovery; computation and dynamics.

Location–The conference will take place at the Centro Internazionale Congressi and Palaffari Firenze located close to the central railway station in the historical and monumental area of Florence.

Accommodation–Accommodation will be arranged in hotels of different categories, mostly within walking distances from the

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venue (student dorms will be available). Detailed information and reservation forms for accommodation will be included in the second circular.

Information on the scientific program, accommodation, general arrangements, registration forms and instructions for preparation of abstracts are continuously updated in our web site. Please visit it! Registration can be done on line. Abstract and early registration deadline is March 31, 2000. For further information, please contact: XIX ICMRBS Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi, 7, 50121 Florence, Italy; Fax: +39 - 0552757555 (do not omit the 0); E-mail: ICMRBS@lrm.fi.cnr.it. Or visit the web address at:

http://www.lrm.fi.cnr.it/icmrbs.html

Conference Committees: *Organizers:* I. Bertini, (Florence, Italy) Chairperson; L. Banci (Florence, Italy) Ex. Manager; R. Kaptein (Utrecht, The Netherlands); H. Rueterjans (Frankfurt, Germany); G. Valensin (Siena, Italy). *Assistants to the organizers*: R. Del Conte & I.C. Felli (Florence, Italy); Treasurer: P. Turano (Florence, Italy). International Advisory Board: A.S. Arseniev (Moscow, Russia); C.M. Dobson (Oxford, U.K.); S. Forsen (Lund, Sweden); G. Govil (Bombay, India); A.M. Gronenborn (Bethesda, USA); C.W. Hilbers (Nijmegen, The Netherlands); J.S. Hyde (Milwaukee, USA); C. Ho (Pittsburgh, USA); M. Kainosho (Tokyo, Japan); J.F. Lefevre (Strasbourg, France); J.L. Markley (Madison, USA); A. McDermott (New York, USA); K. Möbius (Berlin, Germany); R.S. Norton (Parkville, Australia); S.J. Opella (Philadelphia, USA); M. Rico (Madrid, Spain); J. Seelig(Basel, Switzerland); B.D. Sykes(Edmonton, Canada); W. Tang (Nanjing, China); G. Varani (Cambridge, U.K.); A. Walker (Tucson, USA). *National Organizing Committee*: Coordinator: A. Rosato (Florence, Italy); S. Aime (Torino); R. Basosi (Siena); R. Bazzo (IRBM); F. Conti (Roma); A. Di Nola (Roma); A. Lai (Cagliari); S. Mammi (Padova); B. Maravigila (Roma); C. Marchioro (Glaxo); G. Martini (Firenze); H. Molinari (Verona); V. Pavone (Napoli); A. Perico (CNR, Italy); F. Podo (Ist. Sup. Sanita); A. Rigo (Padova); A.L. Segre (CNR); A. Spisni (Parma); M. Tato' (Pharm.& Upjohn); P.A. Temussi (Napoli); A. Tomasi (Modena); A. Tramontano (IRBM); F. Uggeri (Bracco); L. Zetta (CNR). *Chairperson of Local Organizing Committee:* R. Pierattelli (Florence, Italy).

POSITIONS AVAILABLE & WANTED

POST-DOC POSITION AVAILABLE at NIEHS/NIH

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

TWO POST-DOCTORAL POSITIONS OPEN at CORNELL

I currently have two openings for postdoctoral associates in my research group. The areas of research will include: 1) Biophysical Studies of Model and Biological Membranes and Dynamic Structure of Membrane Proteins by Modern ESR; 2) Far-Infrared ESR Studies of Molecular Dynamics in Liquid Crystals, Polymers, and Biological Systems; 3) Two-Dimensional Pulsed ESR Studies of Molecular Dynamics in Liquid Crystals, Polymers, and Biological Systems. Interested individuals should contact: Professor Jack H. Freed; B52 Baker Laboratory of Chemistry & Chemical Biology; Cornell University, Ithaca, NY 14853-1301; e-mail: jhf@msc.cornell.edu. Applicants should be prepared to furnish a complete CV and at least two letters of recommendation.

EQUIPMENT & SUPPLIES EXCHANGE

EPR INSTRUMENT WANTED

Searching for an EPR instrument in good working condition with variable temperature attachements. Contact Dr. Horia Caldararu, Romanian Academy, Institute of Physical Chemistry "I.G.Murgulescu", 77208 Bucharest, Romania, FAX: 40-1-3121147; E-mail: hcaldararu@chimfiz.icf.ro or hcaldararu@pcnet.pcnet.ro.

WANTED: USED BRUKER or VARIAN MAGNET

We are looking for a used Bruker or Varian magnet (with or without power supply). If you (or someone you know) have one which is sitting there collecting dust, please let me know. We will be happy to have it for a reasonable price. Please contact Dr. Jim Liu, Dartmouth Medical School, ☎: 603-650-1784; e-mail: jim.liu@dartmouth.edu.

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- 5-(N-oxylo-tetramethyltetrahydropyrid-4-yl) thyophene-2-al

- 2,6-dimethylenecyclohexanone substituted by 6-(N-oxylo-tetramethyltetrahydropyrid-4-yl) thyen-2-yl residues at both alpha-carbon atoms
- 4-chloro-4-nitro-TMP-N-oxyl

Small quantities of the following compounds are also available:

- 4-bromo-4-nitro-TMP-N-oxyl
- 1,4-di-TMP-butaine-bis-N-oxyl

For information about obtaining any of the above compounds, contact: A.E. Myshkin, Inst. Biochem. Phys., Russian Acad. Sci., Kosygin St. 4, 117977 Moscow V-344, Russia; E-mail: chembio@glas.apc.org.

FOR SALE: BRUKER ESP-300 RADIO-SPECTROMETER

The instrument is intended for investigation of materials by means of electronic paramagnetic resonance (EPR). It was purchased from Bruker Analytische Messtechnik GMBH by St.Petersburgs quartz-glass factory "Stekvar" in 1989 and was installed in 1990 (tested in April 1990). But it was not used at all, because since that time this research activity was stoped at "Stekvar". It was not moved. Now the instrument is working completely. So, the instrument seems like new. This ESP-300 have maximum specification (for example, there is helium low temperature additional device provided by Oxford Instruments). This instrument is provided with system for double and triple resonance. There are some spare parts. System # is ZD 698. The instrument's technical details are: 1) it works in X-band (frequency: 9.79GHz); 2) spare cavities: ER 4111VT, ER 4114 HT, ER 4105 DR; 3) NMR magnetometer is ER 035 M with ESR in cavity probe; 4) microwave bridge is ER 044 MRDH; 5) temperature range from 3.5 K (Oxford Instruments helium low temperature unit); 6) double & triple resonance system. For further information, contact Prof. Roman Eismont, E-mail: empire@peterlink.ru; ☎: 7-812-249-02-95; FAX: 7-812-249-51-14; Regular mail: 6 Shafirovsky Avenue, St. Petersburg 195273 Russia.

AVAILABLE: ISOTOPE-CONTAINING SPIN PROBES

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

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WANTED: MICROWAVE BRIDGE

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

FOR SALE - NMR MAGNETOMETER

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WANTED: TERMINAL/MONITOR

Terminal/monitor for Bruker ECS 106 spectrometer wanted. Contact: Lon B. Knight, Jr., Furman University, Department of Chemistry, Greenville, SC 29613, USA; ☎: 1-864-294-3372; FAX: 1-864-294-3559; E-mail: lon.knight@furman.edu.

AVAILABLE: VARIAN COMPONENTS and MAINTENANCE

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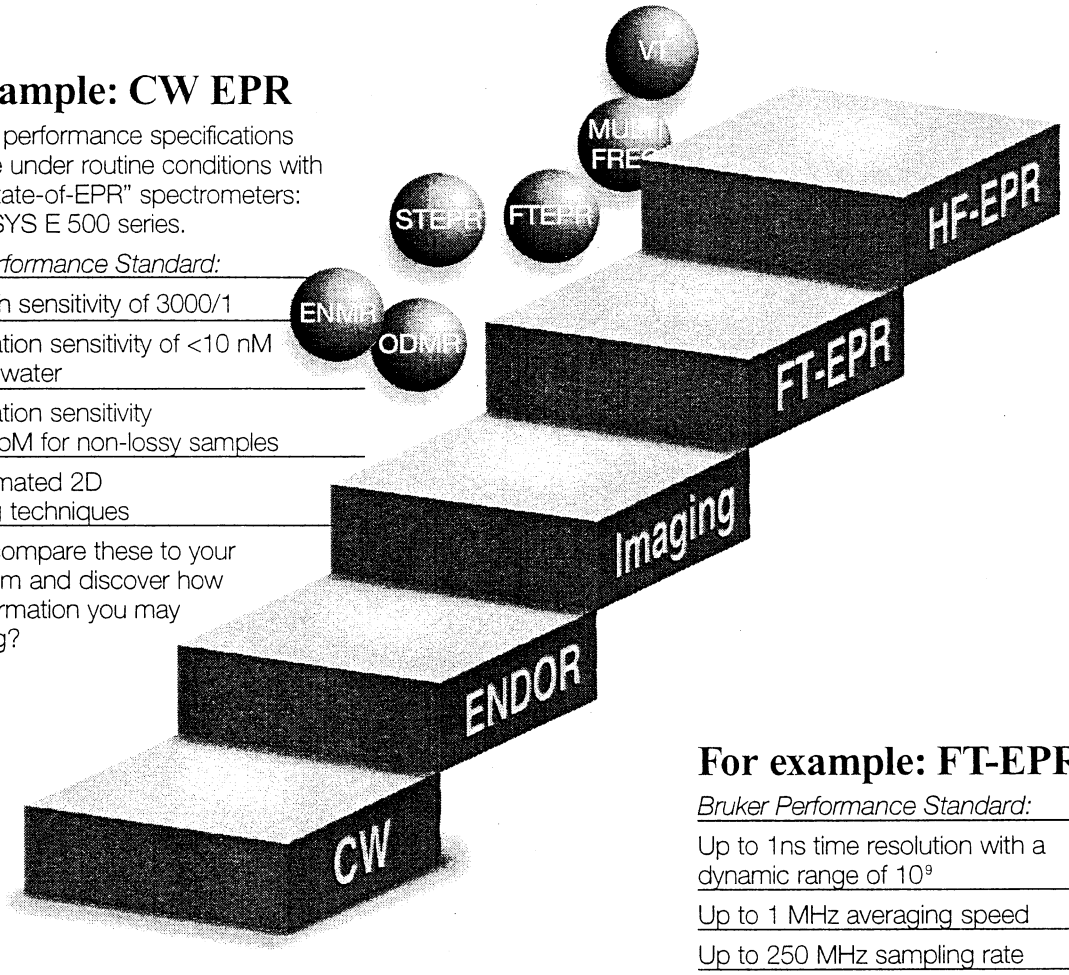

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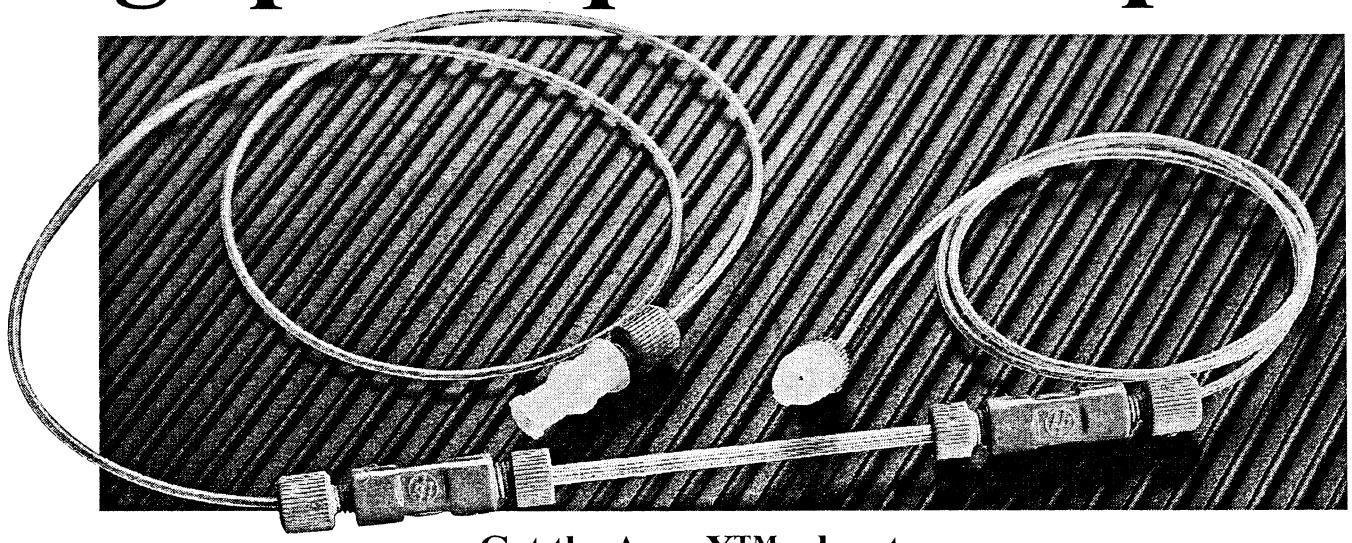

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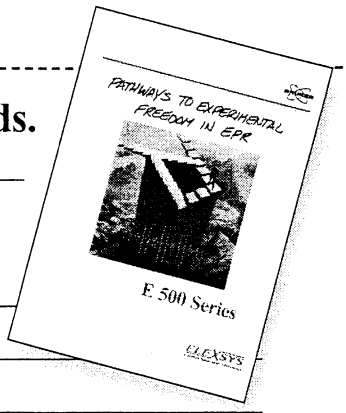

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Department _____

Address _____

City _____ State/Country _____ Postal Code _____

Phone/ext. _____ fax _____ email _____

3) NMR Gaussmeter.

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

NEED HELP in DESIGN and CONSTRUCTION of EPR ELECTRONICS?

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

AVAILABLE: TWO IBM 9000 COMPUTERS

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

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

AVAILABLE: USED VARIAN EPR EQUIPMENT

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

2) Varian ENDOR accessory, with Varian ENDOR cavity.

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

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

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

For details, contact James Anderson, Research Specialties, 5629 N. Maplewood, Chicago, IL, 60659, USA; ☎/FAX: 1-773-728-6570.

FOR SALE: VARIAN SYSTEM

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

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

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WANTED: X-BAND BRIDGE

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

E-MAIL INFORMATION AVAILABLE ON WEB

Since e-mail has become a popular means of communication, having correct e-mail addresses is vital. The directory issue helps, but we receive changes almost every day. To assist in communications among EPR researchers, we have put our list of e-mail addresses on the IES WWW. It is updated monthly. Please check your own e-mail address on the Web and tell us if your address should be added or corrected. The WWW address:

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.

IMPORTANT NOTICE: A NEW CONSTITUTION for the INTERNATIONAL EPR (ESR) SOCIETY and the ELECTION of NEW OFFICERS

Following the masthead (next page), there is an Appendix to this issue of the EPR Newsletter. It contains the text of a proposed new constitution for the IES, together with background and a ballot. This is the result of extensive experience by your officers and a great deal of reflection and effort on their part. The officers of the IES are convinced that the revisions will make the business of the Society run much more smoothly and effectively.

It is also time to elect a new slate of IES Officers. A ballot has been included on page 24.

Please read this material and cast your vote by mail or e-mail.

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ABOUT THIS PUBLICATION

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•Editor: R. Linn Belford
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Illinois EPR Research Center (IERC),
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University of Illinois at Urbana, 190 MSB, 506 South Mathews, Urbana, IL, 61801, USA.
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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:

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

APPENDIX

Background and Explanatory Memorandum: Reasons for a Revised Constitution and Why You Should Vote Yes:

Dear Members of the IES:

During my time as Secretary of the Society, it has became apparent that there were several aspects of the Constitution under which we are meant to operate which no longer worked. I have sought therefore to rewrite the Constitution in the hope that we will have a document that will work well for the Society for the foreseeable future and make the task easier for all Office Bearers.

In the first place the Council, which was very important in the early days of the Society, has not functioned as an effective controlling body. For example in one matter on which I sought response from Council Members, only one Member responded out of about 40. The Executive Committee [or just the Executive] has had to act as both Council and Executive in recent years. In the light of feedback from the members of the present Executive, including the Immediate Past President and the Founding President, I am convinced there is agreement the time has come to disband the Council and to transfer its functions and powers to an enlarged Executive.

Since the establishment of the IES Gold Medal and the setting up of an Awards Committee to manage that Award and the subsequent Silver Medals, Young Investigator Award and establishment of Fellows of the Society, it has become increasingly clear that we were no longer functioning with a single Awards Committee, as laid down by the Constitution, but several committees. The time has clearly come for this to be regularised so that the Constitution matches what we know works well. The Awards Conditions and the structure of Awards Committees are included as By-Laws with the provision that variations can be made by a vote of at least five members of the Executive.

Redrafting to Improve Overall Consistency of Constitution:

I have taken the opportunity to undertake a certain amount of redrafting of some clauses in the Constitution to simplify them and to make them more internally consistent. Articles I – III remain as before with some minor amendments only. The acronym EPR is used in preference to ESR in the Constitution.

Major Changes.

Article IV Council and Officers becomes Article IV Executive Committee and Officers. All references to Council have now become references to Executive Committee [or Executive]. The Executive is to be increased to eight members instead of five through the addition of two further Vice-Presidents and the Editor of the EPR Newsletter who will be a non-voting member. The role of the President has been more clearly defined. The three Vice-Presidents are to be chosen on a geographical basis, notionally Asia [or Asia-Pacific], the Americas and Europe [including the UK and Ireland]. As agreed by the Executive, during a three year term the Vice-Presidents will take year long turns as Senior Vice-President so that in the event of resignation, death etc of the President, the designated Senior Vice-President will assume the Presidency. The role of the Treasurer is spelt out more fully with particular reference to annual reporting of audited accounts to the membership through the first EPR Newsletter each year.

There is a new Article VI on Awards which is quite minimal for the details regarding awards have been placed in the By-Laws and these can be changed by decision of the Executive Committee whereas changes to the Constitution require a two thirds majority of those voting. It makes sense to give the Executive discretion where it is to do with the operation of the Society within

its general purposes.

In the light of the new Article VI on Awards, that on Standing Committees becomes Article VII. The number of Standing Committees has been reduced to the Elections Committee and the Awards Committees which have grown up in recent years. The Nominating Committee has been removed and its functions transferred to the Executive as covered in clause 1 of Article VII. This revision also provides a necessary opportunity to consider how to allow for voting by electronic mail, bearing in mind that this may represent for many an unwelcome loss of confidentiality. Voting by ordinary mail will still of course be possible.

With regard to Fees clause 1 [of what is now Article IX] has been extended to require a vote of the membership by simple majority if it is proposed to increase fees by more than 20% and this should happen 12 months in advance.

Article X, Miscellaneous Provisions, has been subject to some minor editing and, in clause 7, inclusion of ballot by electronic mail as an option for amending the Constitution.

Article XI, Affiliation to the International EPR (ESR) Society, has been amended slightly and the original clause 10 regarding fees becomes clause 4 of Article IX as it seemed to be out of place under 'Affiliation'.

By-Laws: Unlike the Constitution, where changes must be approved by a two-thirds majority of members who vote in a ballot, By-Laws may be made [and changed] by the Executive. The By-Laws attached to this proposed new Constitution concern Awards only. Indeed the present Executive decided it was necessary to create a new Silver Award category for Instrumentation starting in 1999 decoupling Physics and Instrumentation. Thus the Physics/Instrumentation Silver Medal is now two separate awards, a Silver Medal for Physics/Materials Science and a Silver Medal for Instrumentation.

This draft revised Constitution has been vetted by the Executive, the Founding President and a number of senior members of the Society. It is our hope that all members will vote for the changes that bring the Constitution into line with what has become necessary practice.

John R. Pilbrow
Secretary of IES
August, 1999

PROPOSED CONSTITUTION OF THE INTERNATIONAL EPR (ESR) SOCIETY

Article I. Name

The name of this Society shall be the International EPR (ESR) Society hereinafter called the SOCIETY or IES.

Article II. Objectives

The objectives of the SOCIETY shall be:

a) To advance and stimulate knowledge of the principles, recent developments, and applications of Electron Paramagnetic Resonance (EPR) or Electron Spin Resonance (ESR) spectroscopy.

b) To communicate information and news about EPR and its applications among its members and to serve as a clearing house on EPR among scientists in academia, government, and industry by means of the official Bulletin or Newsletter of the Society in either hard copy form or accessible through the SOCIETY's Website.

c) To encourage appropriate and useful application of EPR in a wide variety of fields including physics, chemistry, biology, medicine, geology, and other disciplines;

d) To provide a central voice for the EPR community by promoting support for research and development utilising EPR through interaction with other societies, government funding agencies, and international scientific organisations;

e) To stimulate educational programs on EPR and related spectroscopies through organisation of schools, workshops, courses, and seminars;

f) To foster scientific interaction among EPR spectroscopists throughout the world and to engage in any lawful activities which further this end.

g) The SOCIETY is to be international in scope and is to cover the entire range of disciplines that use EPR.

Article III. Membership

1. The SOCIETY shall consist of Regular Members, Student Members, Postdoctoral Members, Associate Members, Emeritus Members, and Institution Members.

a) Regular Members. Any person who has made a personal contribution to the advancement of EPR or its applications shall be eligible to become a Regular Member.

b) Student Members. Any student actively engaged in EPR research or its applications shall be eligible to become a Student Member.

c) Post-doctoral Members. Any person engaged in EPR research or its applications and holding a post-doctoral position shall be eligible for this status of membership for up to three years. The period may be extended to a maximum of six years upon action by the Executive Committee on the basis of an application to the Secretary that documents continuation as a post-doctoral fellow beyond three years.

d) Associate Members. Any person supporting the objectives of the SOCIETY, and who is not eligible as a Regular Member, shall be eligible to become an Associate Member.

e) Emeritus Members. Any person whose professional activities qualify him/her for status as a regular member and who holds emeritus status or the equivalent.

f) Institution Members. Any institution supporting the objectives of the SOCIETY shall be eligible to become an Institution Member.

2. Admissions. Persons satisfying the required conditions may become Members of the SOCIETY, in the appropriate category, on making written application to the Secretary of the SOCIETY and on paying the membership fee established for that category.

3. Rights and Privileges. All Members of the SOCIETY shall have the right to attend any meeting of the SOCIETY and to participate in the discussion, to receive the official communications of the Society, to hold office, and to vote on candidates for office and on matters of policy.

4. Termination of Membership. Membership of the SOCIETY may be terminated by resignation in writing, or, as provided in Article VIII, by non-payment of membership fees.

Article IV. Executive Committee and Officers

1. Executive Committee. The management of the SOCIETY, including its day-to-day operations shall be vested in an Executive Committee, henceforth referred to as The Executive. The Executive shall consist of the President, the Vice-Presidents, who shall be three in number, the Immediate Past President, the Secretary and the Treasurer, being the elected Officers of the SOCIETY, and the Editor of the Official Bulletin or Newsletter of the SOCIETY as a non-voting member. The composition of the Executive shall provide for a balanced international and geographical distribution, as well as a proper balance of researchers in different branches of EPR.

a) The Executive shall seek to meet at least once per year, normally during a suitable scientific conference or at some other time. On-going business may be transacted by mail, which may include electronic mail, between meetings. The Executive will determine its own rules of conduct of business.

b) The quorum for a meeting of the Executive shall normally be four but members unable to attend, having regard to the agenda previously circulated, may give their proxy to the President or another member present.

2. President. The President shall be the chief executive officer of the SOCIETY and shall normally chair meetings of the Executive and any General Meetings of the SOCIETY. The President shall direct the general affairs of the SOCIETY and execute such other duties as many be determined by the Executive or by resolution of a properly constituted General Meeting of the SOCIETY. The term of office of the President shall be three years, and any person may serve only one term as President, except that if one of the Vice Presidents succeeds to the office as a result of the death, disability, or resignation of the President, such service shall not be counted as a regular term..

3. Vice President(s). The Vice Presidents shall be three in number, to provide for a balanced international and geographical distribution, and will carry out any duties assigned by the President and the Executive. The term of office shall be three years. The Vice-Presidents, during their terms of office will, in turn, be designated Senior Vice-President for periods of twelve months, to carry out the duties of the President in the absence of that person. The Senior Vice-President shall immediately assume the office of President in the event of the death, disability, or resignation of the President. The Executive shall determine the order in which the three Vice-Presidents shall take their turn as Senior Vice-President.

4. Immediate Past President. The Immediate Past President shall remain a full member of The Executive for a period of three years following his/her term as President.

5. Secretary. The Secretary shall maintain all the records of the SOCIETY, shall keep the minutes of SOCIETY meetings, and be responsible for the distribution of all essential information to members. The term of office of the Secretary shall be three years, subject to re-election for no more than two further periods of three years.

6. Treasurer. The Treasurer shall have custody of all funds of the SOCIETY, collect all dues and disburse funds in accordance with the direction of the Executive and shall maintain proper books of accounts for the SOCIETY. The Treasurer shall provide an Annual Audited Financial Statement, which shall include reports of funds held on behalf of the Society by all Regional Treasurers, which shall be published in the first Bulletin or Newsletter of the SOCIETY of each year, covering the previous calendar year. The Treasurer shall also ensure requirements relating to incorporation and taxation exemptions are complied with. The term of office of the Treasurer shall be three years, subject to re-election for no more than two further periods of three years.

7. Editor of the Bulletin or Newsletter of the SOCIETY. The Editor of the Bulletin or Newsletter of the SOCIETY, henceforth referred to as the Editor, who

shall be appointed by the President, shall be a non-voting member of the Executive. The term of appointment as Editor will be determined by mutual agreement between the President and the Editor.

8. Nominations for the positions of all Office Bearers are governed under Section VII 2.

Article V. General Meetings

1. General Meetings of the SOCIETY shall be held during suitable scientific meetings at least once every three years. All participants at that scientific meeting may attend and speak at such meetings, and may vote. The President of the SOCIETY, or the President's designate, shall chair any General Meeting.
2. Quorum. The Quorum for a General Meeting shall be at least 20 Members in attendance. By decision of the Executive any matter deemed to be of major impact on the SOCIETY shall be submitted to the Membership for a mail ballot.

Article VI. Awards

1. Awards made by The Society are governed by the By-Laws appended to the Constitution and, apart from clause 2 of this section, may be altered by resolution of the Executive.
2. The President shall have the power of veto over any Award.

Article VII. Standing Committees

1. In addition to the **Executive,** there shall be the following Standing Committees:
   - Elections Committee
   - Awards Committees

   The Executive may appoint other Committees as required. Recommendations concerning Conferences, Symposia, Courses, and Schools shall be the business of the Executive. A majority of a Committee shall constitute a quorum for business. All recommendations of Standing Committees are subject to approval by the Executive.
2. Elections Committee.
   The Elections Committee shall consist of a Chairperson and two other members from different institutions appointed by the Executive to serve for three years. Members of the Elections Committee may not be candidates in the elections as Officers of the SOCIETY. The Elections Committee shall conduct all elections and mail ballots of the SOCIETY. Mail ballots may include use of electronic mail.
3. Awards Committees.
   There shall be a Committee responsible for each of the Awards of the Society. The Committees, appointment to Awards Committees and responsibilities of the Awards Committees are provided in the By-Laws.
   a) No member any of the Awards Committees may be a candidate for any Award of the SOCIETY for which their particular Committee is responsible.
   b) Office Bearers of the Society may not be candidates for any Award of the SOCIETY throughout the duration of their appointments.

Article VIII. Elections

1. Nominations for all positions of Office Bearers shall be made by the Executive that shall have regard to geographical and international distribution of nominees. Nominations may also be made by at least ten paid-up members of the Society, in writing to the Secretary, and received by a date specified with appropriate notice in the official Bulletin or Newsletter of the SOCIETY. Where there are one or more nominations for any position, the Elections Committee shall conduct the election according to the provisions following in clauses 2 and 3. The Members may vote on ballot papers distributed to them by the Secretary. The ballot papers shall be returned to the Office of the SOCIETY in signed, sealed envelopes by mail. Mail ballots must be received prior to a date specified by the Secretary after consultation with the Elections Committee. Alternatively, Members may vote using electronic mail and should send their vote directly to the Chair of the Elections Committee by the closing date for the election.
2. On receipt of all the ballots for an election, the Secretary shall turn over the ballots to the Elections Committee, which shall open the ballots, tally the votes, including those communicated by electronic mail, and prepare a report of the election, which shall be circulated to members of the SOCIETY.
3. Elections will be held every three years. In the event that an Office of the Society becomes vacant due to any cause, the Executive shall be responsible to find a replacement for the position who shall serve until the next normal election for that position.

Article IX. Fees

1. Fees. The fees (annual subscriptions) for the various membership categories of the SOCIETY shall be determined by the Executive except that proposed increases of more than 20% shall be put to a ballot of all Members 12 months in advance. Members may vote on ballot papers distributed to them by the Treasurer or by e-mail. The ballot papers shall be returned to the Office of the SOCIETY in signed, sealed envelopes by mail by the closing date. Those members who wish to vote using electronic mail may do so by sending their vote to the Office of the SOCIETY by the closing date for the ballot.
2. Waiver of Fees. The Treasurer may waive the membership fee of a Member for good reason. If because of currency restrictions in a Member's

country, Members may have the alternative option to pay their dues in the currency of their country or region to a Regional Treasurer in that country or region who has been appointed by the SOCIETY.

3. Non-payment of Fees. A Member who has not paid the appropriate membership fee by three months after the expiration of the membership period shall be sent a notice of pending termination of membership. If the fee has not been paid by six months after the expiration of the membership period, that person shall cease to be a Member of the SOCIETY. The official Bulletin or Newsletter of the SOCIETY will continue to be sent, or be available electronically, for a period of 12 months whilst efforts are made by the Treasurer to encourage the person to reinstate their membership and to pay any outstanding fees.
4. All members of the Society in developed countries shall pay the standard membership fee (or its local equivalent) per annum. The Treasurer is empowered to set lower levels of fees from those countries or regions for which payment of the full membership fee would cause undue hardship to Members upon application from an appropriate group of Members or intending Members. Members in countries or regions who benefit from this arrangement will receive the full privileges of membership notwithstanding. It will be the responsibility of the Executive to monitor the situation from time-to-time and to pursue the long-term aim for all members to pay the full fee.

Article X. Miscellaneous Provisions

1. Incorporation. The Council may arrange for the SOCIETY to be incorporated in a particular country or state, if it is deemed advantageous to do so. If, for the purposes of incorporation, the SOCIETY requires a Board of Directors or Trustees, then the members of the Executive shall be the Directors or Trustees.
2. Office of the SOCIETY. The Office of the SOCIETY shall be established at an address determined by the Executive.
3. The Financial Year of the SOCIETY shall be the same as the calendar year.
4. Audit. The accounts of the SOCIETY shall be reviewed annually by appropriate independent professionals. A report shall be presented to the Council and reported to the membership in the official Bulletin or Newsletter of the SOCIETY.
5. Divisions. The Executive may approve the formation of Divisions to encompass specialised areas of scientific interest within the EPR field, and shall determine the conditions of operation of such Divisions.
6. Affiliations. The SOCIETY may maintain affiliations with other appropriate organisations as determined by the Executive and governed by Article XI.
7. Amendments. Any provision in the constitution may be amended, or repealed by two-thirds majority of the Members casting ballots in a mail ballot (which may include electronic mail).
8. By-Laws. By-Laws, which define procedures that may be required but which are distinct from the Constitution, may, from time to time, be changed or established by five members of The Executive voting in favour.
9. Dissolution. The SOCIETY may be dissolved by a two-thirds majority of those Members casting ballots in a mail ballot (which may include electronic mail). The assets of the SOCIETY will be distributed in a manner determined by the Executive and in accordance with the provisions of the Articles of Incorporation, in a manner that is consistent with the non-profit status of the SOCIETY.

Article XI. Affiliation to The International EPR(ESR) Society

1. Affiliation to The International EPR(ESR) Society can be applied for by any local EPR/ESR Society already in existence or which is about to be formed.
2. In any affiliation The International EPR(ESR) Society remains the sovereign Society, and the affiliated Society shall be subject to all of its rules and By-Laws. It may, if so wished, establish further rules of its own.
3. The object of affiliation is to allow local societies to benefit from being associated with the world-wide EPR/ESR community represented by The International EPR(ESR) Society, and from its contacts, publications, publicity and advertisements.
4. The role of the affiliated society is to extend the influence and availability throughout the world of The International EPR(ESR) Society, and to provide those services most appropriate to the local membership, for example in helping to arrange Conferences and Summer Schools.
5. In accepting affiliated societies, The International EPR(ESR) Society shall be mindful of their possible impact on similar societies already established in the same general area of the world. No Society will be accepted as an Affiliated Society which might affect the well-being of pre-existing Affiliated Societies, or the interests, including financial interests, of The International EPR(ESR) Society itself.
6. The decision as to whether to apply for affiliation must be made by the local Society under its own rules and regulations.
7. The local Society will normally be responsible for the dissemination of information concerning The International EPR(ESR) Society to its members and for facilitating communications of individual members with The International EPR(ESR) Society.

8. To be accepted as an Affiliated Society, at least one half of the members of the local society should be belong to The International EPR(ESR) Society. However, membership of a local Society by an individual is not a prerequisite for membership of The International EPR(ESR) Society.
9. Each Affiliated Society is required to provide a local Treasurer responsible for collecting the dues from its members in local currency and transferring the total in a single currency exchange at least once a year to the Treasurer of the International EPR Society.
10. All publicity for Conferences, Summer Schools or other activities arranged locally will be published free of charge in the Official Bulletin or Newsletter of The International EPR(ESR) Society.
11. The International EPR(ESR) Society will be pleased to allow its name to be used in assisting the organisation and funding for such meetings. Direct financial support will not be available from the IES The International EPR(ESR) Society. The organisers will be able to request information from The International EPR(ESR) Society database to aid in the arranging and advertising such meetings.

End of Constitution

BY-LAWS

Awards

1. A Gold Medal shall be awarded, normally annually, for distinguished contributions to EPR (ESR) Spectroscopy.
2. Four Silver Medals shall awarded, normally annually, for significant contributions to EPR (ESR) Spectroscopy in the areas of Biology/Biomedicine, Chemistry, Physics/Materials Science and Instrumentation.
3. A Young Investigator Award shall be made, normally annually, for outstanding contributions to EPR (ESR) Spectroscopy by a young scientist in any of the categories listed in clause 2. Nominees should be under the age of 35 years and will ordinarily be at the post-doctoral level. Only in exceptional circumstances will either doctoral candidates or junior faculty members be considered for this Award.
4. Fellowship of the Society may be conferred on individuals who have made influential and distinguished contributions to the practice of EPR (ESR) Spectroscopy and its welfare over a long period.
5. All nominations are to be sent to the President.
6. The President, the Vice-Presidents and the Immediate Past President shall together be responsible for preliminary vetting of nominations, to ensure that inappropriate nominations are not pursued and that overlap between medal categories is dealt with before forwarding nominations to the separate Awards Committees.
7. Nominations shall be invited from all IES Members via the official Bulletin or Newsletter of the SOCIETY.
8. Nominations may also be sought by the Executive from one or more kindred Societies as determined from time to time.
9. All nominations must be accompanied by a 100-150 word citation in support of the nomination and, in the case of the Young Investigator Award, nominees will be asked to provided copies of two recent published papers which in their judgement represents their best work.
10. No Award Committee Member may vote on the nomination of a collaborator or member of their own research team. Appointment to Awards Committees is governed by Article VII, Sec. 4.
11. The Executive may, at its discretion, liaise with other Award Committees and communicate, in confidence, names of those under consideration for the IES Gold Medal award in any year.

It is noted that these By-Laws are subject to Article VI Sec. 2 which states "The President shall have the power of veto over any Award".

Awards Committees

1. Committees for Silver Medal Awards, each consisting of a Chairperson, and three other members, shall be appointed by the Executive.
2. The Gold Medal Award Committee shall consist of a Chairperson, to be appointed by the Executive, and the Chairpersons of the Silver Medal Award Committees as ordinary members.
3. Membership of all Awards Committees shall be for a period of three years. In the case of Silver Medal Committees, terms of office will be staggered to ensure turnover of one ordinary position every year. It shall be the responsibility of the Secretary to advise members of Awards Committees as to their terms of office.
4. Members of all the above Awards Committees may be re-appointed for only one additional three-year term.
5. The Committee responsible for the Young Investigator Award and the appointment of Fellows of the Society shall consist of The President, the Vice-Presidents and the Immediate Past President.

End of Bylaws

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EPR NEWSLETTER

Volume 10, Number 3 Page 1 1999

From the Editor—

The EPR Newsletter is published by and for the members of the International EPR(ESR) Society (IES). An issue is produced and sent to IES members about four times per year. Occasionally, however, a public issue is produced and is distributed to about 4000 people worldwide who may have interest in some aspect of electron paramagnetic resonance (EPR, ESR, EMR) or related spectroscopies such as ferromagnetic resonance (FMR) or dynamic nuclear polarization (DNP). This is such an issue. To those recipients who are not now members of the IES: We hope that you will take a look at this sample issue, see how useful the EPR Newsletter and membership in the IES could be for you, and join the Society. The annual membership dues are extremely low, ranging from the equivalent of US$5 for student members to US$30 for full members, and there are regional treasurers around the world so that you can conveniently pay in your own currency. Members in soft-currency countries or others who would have severe difficulties in paying the regular dues may apply to the IES Treasurer for special consideration. The IES Web site has information about the Society, including a full copy of its new Constitution. Point your internet browser to **http://ierc.scs.uiuc.edu/IES.html** *. For instructions on joining, renewing membership, or updating membership or contact information, see page 22 of this issue.*

A new Directory issue is coming. *Periodically, we publish a members-only issue of the EPR Newsletter including a Directory of not only the IES members as well as the others in our database. The next issue (Volume 10, Number 4, 1999) will be a Directory issue listing institution or company affiliations, mail and e-mail addresses, telephone and Fax numbers, and information on scientific interests. This list is very useful to many colleagues, but it needs to be accurate and up to date. Please inform us if there is a possibility that our contact or other information for you may be incorrect, out-of-date, or incomplete.*

Important - Deadlines for receipt of material for publication: *If you wish to submit any material (notices of conferences, letters to the editor, articles, tips or techniques, reports on conferences, etc.) for forthcoming issues of the EPR Newsletter, please be sure that your submission arrives before the deadline. This is particularly inportant for time-sensitive items such as meeting announcements.* ***The next deadline is January 31, 2000. Items received on or before that date will be considered for inclusion in Volume 11, Number 1.***

Linn Belford, Urbana, Illinois, USA

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

FELLOWS OF THE INTERNATIONAL EPR(ESR) SOCIETY

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- BREBIS BLEANEY
- CLYDE HUTCHISON
- ALEKSANDR PROKHOROV
- GEORGE FRAENKEL
- KARL HAUSSER
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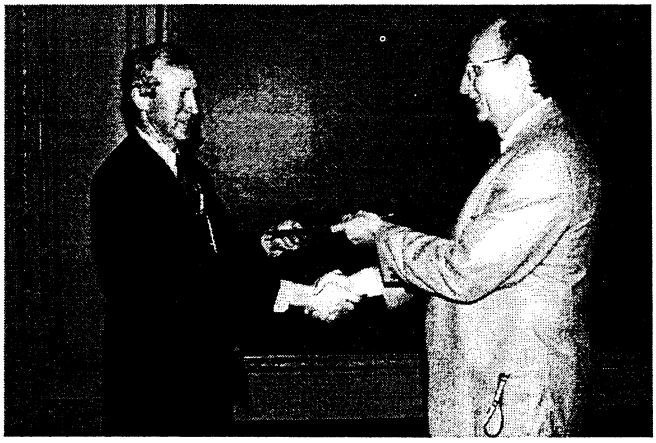
- SAMUEL WEISSMAN
- CHARLES SLICHTER
- JOHN WEIL
- DAVID WHIFFEN
- MELVIN P. KLEIN
- HANS CHRISTOPH WOLF

1999 IES Medal Winners

Professor Brian M. Hoffman, IES Gold Medal Winner for 1999—

Professor Brian Hoffman of Northwestern University has pioneered many applications of EPR as a central tool for determining the structure and function of metallo-enzyme active sites. More than 20 years ago he recognised that to obtain necessary resolution of the interactions for most nuclei in the neighbourhood of the active sites of metalloproteins, ENDOR would be required. More recently this has involved pulsed ENDOR at Q-band, particularly to improve measurement of the 'through space' anisotropic dipolar term. Thus distances well beyond the coordination sphere can be measured to bound substrates and inhibitors which are not coordinated to the metal ions at active sites. Hoffman and his



Brian Hoffman receiving the IES Gold Medal from John Pilbrow at the 22nd International EPR Symposium in Denver on August 2, 1999. *(Photo: Peter Doan)*

IN THIS ISSUE

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

group have investigated many enzymes including ribonucleotide reductase, cytochrome P450, cytochrome c oxidase, chloroperoxidase, ferredoxins and hydgrogenase with an emphasis on the elucidation of electron transfer processes. In 1996 he received the Bruker Prize of the Royal Society of Chemistry ESR Group in the UK. In awarding this year's IES Gold Medal to Brian Hoffman we are honouring an acknowledged leader and pace setter in the application of EPR methods to the study of the structure and function of metallo-enzymes.

The Gold Medal, Certificate and Citation were presented by John Pilbrow, IES Secretary, during the 22nd International EPR Symposium in Denver, 2nd August 1999.

Professor Jack Peisach, 1999 IES Silver Medalist for Biology/Medicine—

Professor Jack Peisach from the Albert Einstein College of Medicine has devoted his career to understanding the chemistry of metal ion cofactors in enzymes and drugs. Collaborations with both Dr. Bill Mims and the late Dr. Bill Blumberg, of the Bell laboratories, on low temperature EPR spectroscopy of metallo-enzymes and transition ion model complexes proved particularly fruitful and led to many novel applications of CW- and pulsed-EPR spectroscopy to problems in metallo-biochemistry. Peisach's role in providing important applications and focusing on the chemical questions associated with them fueled the development of new EPR methods and data analysis strategies. These are the well-known Blumberg-Peisach plots for copper (II) and truth tables for heme proteins that have been widely used to gain an immediate insight regarding metal ligation structure directly from spectral data. Together

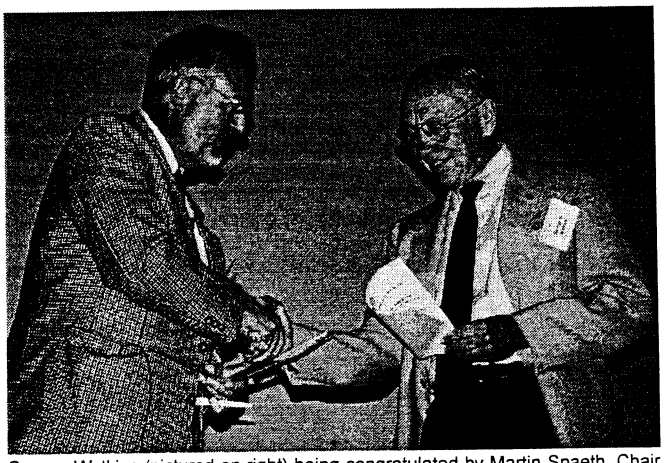
Jack Peisacn receiving the IES Silver Medal for Biology/Medicine from John Pilbrow at the 22nd International EPR Symposium in Denver on August 2, 1999. *(Photo: Peter Doan)*

with Mims, Peisach played a major role in developing Electron Spin Echo Envelope Modulation and Linear Electric Field Effect measurements for applications to biological problems. He continues to be a leader in the application of these methods to problems in bioinorganic chemistry and this is recognised in the Award of the 1999 Silver Medal for Biology/Medicine.

The Silver Medal, Certificate and Citation were presented by IES Secretary John Pilbrow during the 22nd International EPR Symposium, Denver, 2nd August 1999.

Professor George D. Watkins, 1999 IES Silver Medalist for Physics/Materials Science—

The Award is presented for outstanding work on the investigation and understanding of point defects in semiconductors during several decades. George Watkins has been a pioneer in applying electron paramagnetic resonance



George Watkins (pictured on right) being congratulated by Martin Spaeth, Chair of the IES Silver Medal Committee for Physics/Materials Science in Berkeley on July 26, 1999.

to the identification of point defects in solids, first in alkali halides, then in semiconductors, in particular silicon, and also in II-VI and III-V semiconductors. He is known for the study and identification of numerous radiation damage centers created by electron irradiation *in situ* at low temperatures. His work is characterised not only by excellent experiments, but in particular by close collaboration with theoretical physicists and his own theoretical work. For example, amongst a lot of key contributions, his theoretical interpretation of the silicon vacancy and contribution to the understanding of so-called "negative U" centers has become a model for much subsequent work. George Watkins is to be regarded as leader in the field of semiconductor defects and materials science problems related to this.

Professor Watkins worked for many years at the General Electric Research Laboratories and spent the latter part of his career at Lehigh University. He is a Member of the National Academy of Sciences of the USA.

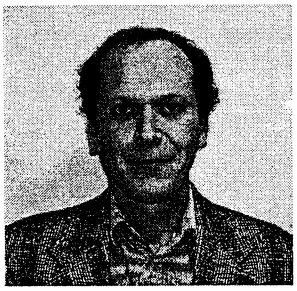
The presentation of the Award was made by Professor Martin Spaeth, Chair of the Silver Medal Committee for Physics/Materials Science, during the Conference on Defects in Semiconductors, Berkeley, California on July 26th. Regrettably neither the Medal nor the originals of the Certificate and Citation could be sent to Berkeley in time for the presentation.

Professor Yuri D. Tsvetkov, 1999 IES Silver Medalist for Chemistry—

Yuri Tsvetkov is winner of the 1999 Silver Medal for Chemistry for his outstanding contributions to the development of electron spin echo spectroscopy and applications. His research has covered many fields of radiation chemistry and photochemistry. In particular he is noted for studies of spatial distributions of free radicals in irradiated solids, electron polarization transfer in liquids, spatial peculiarities of elementary photochemical reactions and molecular dynamics of spin labels in liquids and glasses. Tsvetkov's contributions to investigations of modulation phenomena in electron spin echo envelope modulation in poly-oriented systems have been widely applied to investigations of the structure of traps for free electrons, atoms and radicals in irradiated solids, the structure of the solvation shell for organic radicals and bonding of radicals adsorbed on surfaces. He is the author or co-author of several books on pulsed EPR, that with Dikanov being most well known in the West. Since 1993 he has been Director of Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences in Novosibirsk. In 1997 he was elected to full membership of the Russian Academy of Sciences.

The Award of the Silver Medal, Certificate and Citation will be presented by John Pilbrow, IES President-Elect, during the 2nd Asia-Pacific EPR Symposium in Hangzhou, China, 31st October – 4th November 1999.

Dr. Ilya Shkrob, 1999 IES Young Investigator—



Ilya Shkrob, 1999 Young Investigator

Dr. Ilya A. Shkrob is recognized for his exceptional creativity and accomplishments in the study of energy transport and charge dynamics in condensed phases. He is an expert practitioner of all the advanced EPR methods, both CW and pulsed, as well as optically detected EPR, which he has applied to a broad range of studies of radical ions and radicals. In addition to his magnetic resonance expertise, Dr. Shkrob uses lasers to study fast chemistry by conductivity and optical detection. The objective of Dr. Shkrob's work continues to be an understanding, at a fundamental level, of the interaction of ionizing energy with molecular liquids and amorphous solids. His studies on the generation and structure of radiation-induced defects in oxide glasses provide new insights into the issues of radiation stability of glass forms that are used for long-term storage of radioactive waste. His recent work has addressed novel chemistry of excited radical cations and ultrafast hole transport in nonpolar liquids. These results are important to everyone interested in electron transfer reactions as such processes are widespread in chemistry and in bioenergetics. Shkrob received his Ph.D. from the Institute of Chemical Physics of the Russian Academy of Sciences in Moscow, under A.L. Buchachenko and V.F. Tarasov. He worked in a postdoctoral capacity at Oxford, UK; Queen's University, Canada; and at Argonne National Laboratory, USA. He is an author of more than 60 publications. Dr. Shkrob is currently an assistant chemist in the Radiation and Photochemistry Group of the Chemistry Division of Argonne National Laboratory.

Dr. Marion Thurnauer

IES FELLOWS 1999

Dr. Melvin P. Klein, IES Fellow 1999—

Mel Klein has contributed greatly not only to the EPR methods for which we honor him with Fellowship of the International EPR Society, but also to NMR, Mossbauer, X-ray and optical spectroscopies. His early love of radio technology, pre-WWII engineering training at the University of Denver, and wartime and subsequent involvement in rf and other instrumental technologies equipped him to introduce digital signal averaging, the use of fluorescence X-ray detection in EXAFS, and the advancement of coherent Raman Beat EPR. Mel worked at both the Berkeley and Livermore National Laboratories, and was a key figure in Berkeley's "Round House" after being recruited by Melvin

Melvin Klein, IES Fellow

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Calvin in 1963. In the 60's and 70's, Mel worked on both metal and radical paramagnetic systems, both at Berkeley and on sabbatical with Bill Blumberg and colleagues at the Bell Labs. In recent years, by creative use of X-ray spectroscopy and advanced EPR methods, Mel has pioneered major advances in our understanding of how plants oxidize water to form molecular oxygen. EPR aspects of this work include advancing our understanding of the mixed valence Mn complexes, the discovery of new signals and spectral features presented by the Mn cluster at the core of the oxygen evolving complex, introduction of pulsed EPR methods to explore the cluster nuclearity and ligation, and the use of parallel polarization EPR to examine non-Kramers doublets of the Mn cluster and synthetic analogs.

The Award was announced at the 22nd International EPR Symposium, 1-5 August 1999 in Denver. A formal presentation will take place at a future event.

Professor Martyn Christian Raymond Symons FRS, IES Fellow 1999—

Studies of reaction mechanisms at Battersea Polytechnic, London, in the 1950's led Martyn Symons to see the importance of EPR in Chemistry. Joining the Chemistry Department at the University of Southampton in the late 1950's, he collaborated on EPR with David Ingram of the Electronics Department, and the mathematician, D.S. Schonland. Martyn's collaborative style impacted on his many students, among them Alan Carrington FRS and Peter Atkins. In 1960 he was awarded a D.Sc. from London University and also appointed to the Chair of Physical Chemistry at Leicester. In an amazingly productive era spanning more than 30 years at Leicester, Symons applied EPR to inorganic radicals produced by radiolysis (summarised in his monograph with Atkins), metal-ammonia solutions (with R. Catterall), transition metal compounds, and silver halides. His other interest was in solvation and remarkably his most cited papers are in that field. Since retirement, Martyn has been Visiting Professor at de Montfort (Leicester), the University of Essex (1993-5), and London University. He was elected Fellow of the Royal Society (1985). He was the first Bruker Lecturer (1986), Robinson Memorial Lecturer of the Royal Society of Chemistry (1987) and Whelan Lecturer at the University of Saskatchewan (1997). Despite personal tragedies, keen interests in piano playing and watercolour painting go hand-in-hand with his on-going interests in science. Martyn Symons is one of the most cited scientists of current times and he has authored or co-authored approximately 1300 publications.


Martyn C.R. Symons, IES Fellow

Arrangements will be made for a formal presentation of this Award.

Prof. Dr. Hans Christoph Wolf, IES Fellow 1999—


Hans Christoph Wolf, IES Fellow

Just three years after Feher's first seminal article on ENDOR, Wolf and Horst Seidel in an investigation of color centers, reported room temperature ENDOR for the first time. In an outstanding career that followed, Wolf pioneered the combination of optical spectroscopy and magnetic resonance, including EPR, NMR and ENDOR, to a variety of studies of organic aromatic molecules in the solid state, work that depended on the ability to grow very pure single crystals. He discovered the mini-exciton in naphthalene pairs found in mixed crystals of protonated naphthalene doped into perdeuterated naphthalene and in anthracene which have served as a paradigm and model system for numerous studies involving excitons on linear chains, pair excitations and the primary donor in the photosynthetic reaction center. Other major discoveries include: the first ENDOR from light induced triplet states (with a student P. Ehret); an optical nuclear spin polarization mechanism whereby the nuclear spin is polarized through the light-induced electron spin polarization in triplet state molecules in the solid state (with K.H. Hausser); and the first determination of the fine structure tensor of a carotenoid molecule from light-induced transient CW-ESR studies of ß-

Carotene single crystals (with G. Kothe). These achievements have been shared with many co-workers and students, six of whom have moved on to Professorships.

Arrangements will be made for a formal public presentation of the Award.

Professor Arnold Hoff, 1999 Voevodsky Award Winner

The Voevodsky Award is granted for a significant contribution in investigation of elementary chemical processes. The achievements of Arnold Hoff in this field are well known. Over the years, his research has been focussed on primary processes in photosynthesis, structure/function relationship in photosynthetic reaction centers, site-directed mutagenesis of bacterial reaction centers. Experimental methods used in his research include EPR (routine, time-resolved, electron spin echo, high-field and optically-detected), laser flash spectroscopy, magneto-optical resonance techniques.

1999 Voevodsky Winner Arnold Hoff

Arnold successfully used Optically-Detected Magnetic Resonance (ODMR) to investigate triplet states in photosynthetic preparations. He discovered that detection via the absorption offered significant advances in sensitivity, and, in detecting microwave-induced Triplet-minus-Singlet absorbance difference spectra. This approach continues to be used for elucidating the structure of the primary donor and its environment in photosynthetic reaction centers.

He was, in a collaboration with Peter Hore, Oxford University, first to propose the Correlated Radical Pair mechanism as the process producing the Electron-Spin Polarized signals in bacterial and plant photosystems. This concept is now universally accepted, and has proved an important means to determine exchange interactions between the primary reactants from time-resolved EPR spectra, magnetic field effect measurements and Reaction Yield-Detected Magnetic Resonance. Recently, in collaboration with Institute of Chemical Kinetics and Combustion, he has developed an electron spin echo method to determine very accurately the distance between the members of a photo-induced radical pair using an electron spin echo spectroscopy. In addition, strong photoselection effects were discovered in Electron Spin Polarized EPR spectra recorded with time-resolved EPR. Much work was done on ESEEM of radicals and triplet states in photosynthetic reaction centers. This work provided the first unambiguous evidence on the hydrogen bonding pathways of the acceptor quinones, indicating how their electron transport properties are modulated by the protein matrix.

In addition to the applications of magnetic resonance, he has achieved notable successes in optical investigations of bacterial reaction centers. In collaboration with Martin and Breton, France, the first precise determination was carried out of the charge-separation time of bacterial reaction centers with femtosecond spectroscopy. With Wiersma, The Netherlands, the first holeburning experiment on bacterial reaction centers was done (independently also performed by Boxer, USA), opening the now thriving field of hole-burning in photosynthesis. With the groups of Amesz/Artsma, Leiden, and Shuvalov, Moscow, modified and mutant bacterial reaction centers were characterized with nanosecond and femtosecond spectroscopy, giving evidence for a thermally-activated charge separation in reaction centers, and demonstrating vibrational oscillations participating in electron transport on a femtosecond time scale.

Arnold Hoff is open for cooperation and maintains it with scientists from many countries. This cooperation has turned out to be very fruitful in many cases. A very important condition of these successes is his high professional qualification.

He is deeply involved in numerous administrative, editorial and reviewing work. His *curriculum vitae* includes more than 280 articles in leading international journals and more than 15 chapters in edited books and monographs. He was invited speaker, including numerous plenary lectures, at more than 100 international symposia and conferences and more than 75 seminars; invited guest lecturer at over 15 Universities and Institutes.

Sergei Dzuba
Institute of Chemical Kinetics
and Combustion, Russia

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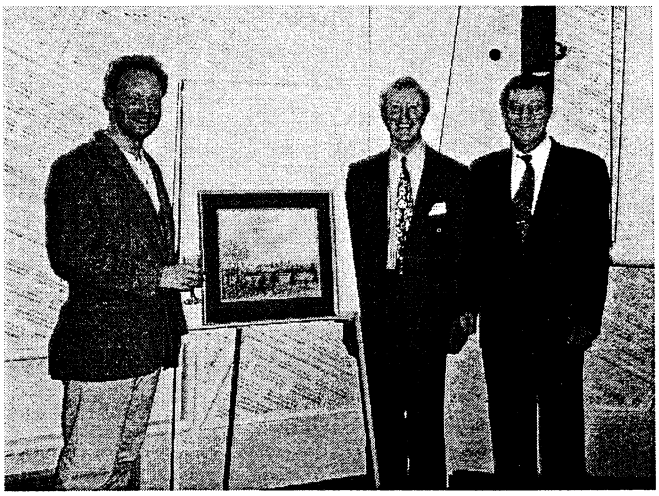
John Pilbrow, 1998 Bruker Award Winner

On March 31st last year, IES Secretary, Professor John Pilbrow, received the 1998 Royal Society of Chemistry ESR Group Bruker Prize and presented the Bruker Lecture to the 31st Annual International Meeting of the Royal Society of Chemistry Electron Spin Resonance Group held at the University of Manchester in the UK. John is Head of the Department of Physics at Monash University, Melbourne, Australia where he has been since 1965.

His lecture was entitled "EPR Spectroscopy – Past History, Present Status, Future Prospects." He covered his introduction to EPR in New Zealand in 1960, reminiscences of the Clarendon Laboratory in Oxford in the early 1960's where he was a graduate student and a historical overview that was relatively unknown to younger members of the audience. Examples drawn from physics, chemistry, and biology illustrated a range of contributions since 1965 at Monash University beginning with the determination of structural information for a range of metal ion dimers and the effects of low symmetry on the EPR spectra of transition ions in crystals and biomolecules. He highlighted important consequences of the usual magnetic field swept EPR spectra such as asymmetric lines for non-crossing levels and for g-strain broadening. These are explained simply by working in the frequency domain, thus avoiding corrections factors previously used. He predicted that the future of EPR spectroscopy would be largely in chemistry and biology and he asserted that high magnetic field and pulsed methods would become commonplace in the 21st Century.

John's prize, a framed watercolour of the dreaming spires of Oxford by contemporary Oxfordshire artist, Ken Manley, was presented by the Chairman of the Royal Society of Chemistry ESR Group, Professor Chris Rhodes. Dr. Dieter Schmalbein, Managing Director of the EPR Division of Bruker AG, Karslruhe (Germany), which provided the prize money, was also present. John presented both Professor Rhodes and Dr. Schmalbein with a Monash Corporate tie. Following the Lecture, Bruker hosted a reception in honour of the prizewinner.



John Pilbrow (center), 1998 Bruker Prize winner, with Chris Rhodes (left) of the Royal Society of Chemistry ESR Group and Dieter Schmalbein (right) of Bruker Analytische Messtechnik. Photo taken 31 March 1998, following Prof. Pilbrow's Bruker Lecture in Manchester.

John was Secretary of the International EPR(ESR) Society from September 1997 – September 1999 and is our newly-elected President. He is also currently President of the Australian Institute of Physics for 1999-2000.

✦ *IES AFFAIRS* ✦

ANNOUNCEMENTS AND REPORTS FROM THE INTERNATIONAL EPR (ESR) SOCIETY

From the Outgoing President—

The IES has been in existence for about ten years. Last year (August) in Berlin at the Joint 29th Ampére 13th ISMAR International Conference on Magnetic Resonance and Related Phenomena, current and past officers of the IES met. At the recommendation of John Pilbrow, we decided that after ten years we should compare how the IES works to how we are expected to work. We quickly resolved to make changes so

that there is a closer correspondence between expectations and realities.

Here are some of the changes that will be implemented as soon as possible. First, John Pilbrow took on the difficult task of rewriting the constitution of the society. The proposed changes in the constitution primarily reflect the reality of how the IES has actually operated during its first ten years versus the plan of operation as outlined in the current, original constitution.

Next, we decided to give actual medals when the IES bestows honors on people. Arrangements have already been made to secure these medals. Naturally, the IES will see that all previous medal winners will receive medals retroactively. In addition, the method of selecting the winners of the awards will be streamlined in the manner to be outlined in the proposed new constitution.

We also suggest the creation of several vice president positions representing different geographical regions around the world. This should provide more effective two-way communications and will, to a significant extent, replace one of the expected roles of the large council.

Additionally, we agreed that the various required operational functions of the IES should be modified. The finances of the IES will be more structured with routine reports submitted frequently to the international treasurer. The group at Illinois founded the EPR Newsletter and has done an excellent job of editing and producing it for over ten years. However, it is a very big chore, and the Illinois group cannot be expected to shoulder this burden forever. From time to time, the Executive Committee including the Editor should from time to time consider whether all or part of this enormous task should be shared or passed on at some point. However, any such transition would be difficult and would need the input and cooperation of many members to build effectively on the high standards that Illinois has established for the Newsletter.

All of the changes outlined above are intended to make the IES function more smoothly and to serve the EPR community better. We hope that you will agree with the proposed alterations and that you will approve of the changes by your vote on the new constitution. The new constitution should be ready to publish in a later newsletter this year to enable the vote to take place. Please feel free to send any comments or additional suggestions to one of the current officers.

James R. Norris

From the Incoming President—

Dear Members,

I shall count it a privilege to serve the Society as its 4th President and I hope I can match the vision and effort of all three past Presidents, Hal Swartz, Keith McLauchlan and Jim Norris. I would like to pay tribute to all of them for the way in which they all ensured the Society remained an important and viable organisation with the primary purpose of providing service to all of the members.

On your behalf I want to thank Jim Norris for his leadership these past three years. I have enjoyed working with him as his Secretary and valued his wisdom at many points. Last March I had the pleasure of staying with Jim and Carol for nearly three days, on my way to the IUPAP General Assembly in Atlanta, and it was good to have time to run through all of the issues to do with the management of the Society and the new arrangements for Awards. Klaus Möbius as Vice-President has always been willing to provide help and advice and the Society has benefited from his quiet wisdom. Thanks are due to Raman Kalyanaraman, who was Treasurer for four years. Keith McLauchlan, as Past President, remained keenly committed to the Society and he was never more than an email message away when advice was required.

In his last Presidential message, Jim Norris has provided a summary of recent activity by the outgoing Executive, in particular the reasons for the new constitution and the benefits that will flow from a more stringent timeline for our activities and functions.

In the two years that I served as Secretary, I have gained a good grasp of the affairs of the Society and I hope that some of the innovations I introduced will make the load easier for all of the incoming Office Bearers – Hiroaki Ohya-Nishiguchi [Vice-President], Haim Levanon [Secretary] and Chris Felix [Treasurer]. As Jim Norris's letter point out the new Constitution will require us to appoint two further Vice-Presidents as part of an enlarged Executive. Nominations will be called for as soon as the new Constitution has been voted in. Linn Belford as the current Editor joins the Executive as non-voting member.

As much as possible I tried to ensure that the Society's Office Bearers were able to meet face-to-face for the

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management of any Society is much easier to achieve when people have a chance to talk things through and to know each other. This is especially important given the international nature of IES. Thus three Executive Meetings were held in 1998 and 1999 and while not everyone could attend all of them, the fact that they took place provided the opportunity to discuss what was working well and what needed improvement. It was out of the meeting in Berlin during the Ampere/Ismar meeting in August of last year that the need for a revised constitution was recognised. Hopefully the votes are coming in to ensure that what we do is consistent with the rules!

Following the Denver meeting last August, taking advantage of the free side-trip London-Tel Aviv-London on my round-the-world ticket, I managed a whole day with Haim Levanon in Jerusalem to discuss the organisation of the Society for the next three years. In two weeks from now I will visit Japan for two days following the 2nd Asia-Pacific EPR Society in Hangzhou, China. Thus Hiroaki Ohya-Nishiguchi and I will be able to discuss the full range of IES business and how to raise the profile of the Society and, in particular, what special role the Vice-President can undertake. Chris Felix, our Treasurer, and I shared an office in Jim Hyde's lab during my sabbatical in Milwaukee twenty years ago. Chris will be an excellent treasurer having taken over many of the day-to-day functions in recent years from Raman Kalyanaraman when his workload made it difficult to attend to IES finances.

It is very pleasing to report that the Society now has a logo and medals for all present and past winners of Gold, Silver and Young Investigator Awards. There is no doubt it was an embarrassment to the Society to award Medals but have no actual medals to present! During the Ampere/Ismar meeting in Berlin last year, Professor Tengiz Sanadze from the Republic of Georgia offered to make some sample medals for us to consider. In so doing he designed the logo which the Executive adopted at the Executive meeting last March in Chicago. The logo was used on the Newsletter for the first time just recently [10/2]. We hope you like it. It looks magnificent on the obverse side of all of the medals. So we are deeply in Tengiz Sanadze's debt.

The first to receive medals at the right time were Brian Hoffman [1999 Gold Medal], Jack Peisach [1999 Silver Medal for Biology/Medicine] last August in Denver. Bill Mims's 1998 Silver Medal for Physics/Instrumentation was presented on his behalf to Jack. Another 12 medals were presented at the Dinner at the Denver Meeting. Recent correspondence from those who have received their medals in arrears by post shows that there is universal pleasure at receiving them at last!

The incoming Executive are considering a schedule of deadlines for awards, Newsletter and finances and I await their responses. Getting our deadlines into the open will make everyone's job a bit easier.

John Pilbrow

From the New Treasurer —

I appreciate the trust placed in me by being elected Treasurer for the Society. I am looking forward to continuing the fine job that Dr. Kalyanaraman has done during his tenure and work to further improve procedures for notification and payment of dues.

Christopher C. Felix

IES Awards —

Call for Year 2000 IES Awards Nominations—

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

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.

The ***IES Gold Medal*** is the premier award of the Society and it stands with the Bruker and Zavoisky Prizes as being one of the three major awards recognising outstanding achievements in EPR. Nominations may be made in any field of EPR, though the Gold Medal Committee will be mindful of the areas of the Bruker and Zavoisky Awards for that year.

Silver Medals: There are four Silver Medals to be awarded annually. These are in the categories of Chemistry, Physics/Materials Science, Instrumentation, and Biology/Medicine.

Young Investigator Awards: There is one Young Investigator award each year. To be eligible, nominees must be under 35 years of age on January 1 of the award year.

Fellows of the Society: The title of Fellow of the Society will be conferred on those who have made truly outstanding contributions in EPR theory and practice. It is intended for particularly distinguished scientists (hopefully, IES members) who are either retired or are close to retirement. As the highest international standards are to be applied to the recognition of those worthy of this distinction, their formal connection with the Society will enhance its own image.

Confidential nominations for all 2000 awards are to be sent directly to the President, International EPR Society, Prof. John Pilbrow, Monash University, Dept. of Physics, Clayton Victoria, Australia 3180 by January 15, 2000. Nominations must include a draft citation of about 150 words on the nominee that may be used in the *EPR Newsletter* if the nominee is selected to receive an award, and sent in an envelope marked "Confidential: to be opened by addressee only." Alternatively, nominations and the accompanying 150 word citation may be sent either as an e-mail text message or as an attachment in RTF format readable on a PC to the following e-mail address: john.pilbrow@sci.monash.edu.au.

Late nominations will not be considered. It is the intention of the Executive to stick to a strict timetable to provide ample time to arrange appropriate award presentations at major conferences later in the year.

Previous IES Awards Winners—

IES Gold Medal: 1992-George Feher; 1993-James Hyde; 1994-Jack Freed; 1995-Sam Weissman (Chemistry); 1996-Kev Salikhov (Physics & Instrumentation); 1997-Harden M. McConnell (Biology & Medicine); 1998-Arthur Schweiger (Chemistry); 1999-Brian Hoffman. ***IES Silver Medals Biology/Medicine:*** 1994-Hal Swartz; 1995-Lev Blumenfeld; 1996-Ron Mason; 1997-Anatole Vanin; 1998-Ed Janzen; 1999-Jack Peisach. ***IES Silver Medals Chemistry:*** 1994-Keith McLauchlan; 1995-Clyde Hutchison; 1996-Klaus Möbius; 1997-Hanns Fischer; 1998-Richard W. Fessenden; 1999-Yuri Tsvetkov. ***IES Silver Medals Physics/Instrumentation:*** 1994-Wojciech Froncisz; 1995-Jan

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Schmidt; 1996-Johann-Martin Spaeth; 1997-Roger Isaacson; 1998-William B. Mims. ***IES Silver Medals Physics/Materials Science:*** 1999-George Watkins. ***Young Investigator Awards:*** 1994-Devkumar Mustafi (Univ. Chicago); 1995-R. David Britt (Univ. California); 1996-Gunnar Jeschke (Univ. Bonn); 1997-Robert Bittl (Techn. Univ. Berlin); 1998-Alex Smirnov (Univ. Illinois); 1999-Ilya A. Shkrob (Argonne National Lab). A listing of the ***Fellows of the Society*** appears on page 1.

Deadlines Set for Newsletter Materials

Henceforth there will be firm and fast deadlines for the receipt of materials for each issue of the *EPR Newsletter*. They will be published in each issue of the newsletter and on the *EPR Newsletter* web page, and the next deadline is:

Volume 11 Number 1: **January 31, 2000.**

THE COMPUTER CORNER

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

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

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

****

Simulating 2-D, [Field-Frequency], Orientation-Selective ENDOR and ESEEM Patterns

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We have devoted considerable effort to devising procedures by which the full hyperfine and quadrupole ($I > ½$) tensors of a hyperfine-coupled nucleus in a frozen-solution sample can be determined. These can be measured by collecting a 2-D, 'hyperfine-selective' ENDOR/ESEEM data set comprised of spectra collected at multiple fields across the EPR envelope, and then comparing them to simulated 2-D patterns. This note describes (briefly), the concepts of orientation selection,[1,2] the programs that have been created to model 2-D ENDOR/ESEEM patterns, and the analysis procedure that uses them. Selected references to an extended review[2] and several recent applications,[3-5] including that to ESEEM,[6] are included.

Orientation Selection

The samples employed in the ENDOR studies of metalloenzymes almost always are frozen solutions and thus contain a random distribution of all possible protein orientations with respect to the applied magnetic field, $\mathbf{B}_0$. From the point of view of the molecules this means that there is an equal probability for the field to have any orientation with respect to the molecular framework. However, this does not mean that all information about the *orientation* of the hyperfine interaction tensors is lost. If a molecule exhibits resolved anisotropic magnetic interactions, namely anisotropic g, hyperfine, and/or zero-field splitting tensors, then the EPR intensity at each fixed applied field arises only from a mathematically well-defined, restricted subset of orientations of the field relative to the molecular framework. This correlation of field and orientation (*orientation selection*) provides a means of obtaining complete hyperfine tensors from ENDOR studies of polycrystalline (frozen-solution) samples.

Consider the EPR spectrum of a center with a rhombic g tensor ($g_1 > g_2 > g_3$) without resolved hyperfine splittings. ENDOR spectra taken with the magnetic field set at either of the extreme edges of the EPR spectrum arise only from those molecules for which the magnetic field happens to be directed along the corresponding g-tensor axis, but the full description of nuclear hyperfine and quadrupole tensors requires more information than is contained in these two single-crystal-like spectra. An ENDOR spectrum obtained using an intermediate g value (magnetic field) is not associated with a single orientation, but it does arise only from those molecules for which the orientation of the field satisfies the relation, $g(\theta, \phi) = g$, where $g(\theta, \phi)$ is the angle-dependent g factor. For each g value this set of orientations can be represented on the unit sphere by a curve, s_g. Each member of a series of ENDOR spectra collected at fields (g values) across the EPR envelope samples a different set of molecular orientations, in analogy to the way that rotating a single crystal in a field samples different individual molecule orientations. Thus, a 2-D, stacked-plot or contour-diagram ENDOR dataset comprised of spectra collected at multiple fields across the EPR envelope is the frozen-solution

analogue of the 2-D orientation-frequency plots collected from dilute single crystals.

We have developed an analysis procedure wherein such a series of orientation-selected ENDOR spectra can be simulated to determine the principal values of the nuclear hyperfine and quadrupole tensors *and* their orientations relative to the g-tensor framework. Ignoring for the moment the existence of a non-zero EPR linewidth (employ a δ-function EPR envelope), the EPR signal intensity at field B, and thus the ENDOR spectrum, arises from those selected molecular orientations associated with the curve on the unit sphere, s_g, comprised of points for which the orientation-dependent spectroscopic splitting factor, satisfies the condition: $g(\theta,\phi) = g$. However, although g is constant along the curve, s_g, the orientation-dependent ENDOR frequencies are not. Thus, the ENDOR intensity in a spectrum taken at g is the summation of the contribution of the selected subset of orientations associated with s_g. This superposition spectrum can be calculated as convolutions over the ENDOR frequencies that arise on the curve, s_g, obtained by an integration of the *area* element along the curve, s_g. In the case of an EPR spectrum that shows resolved hyperfine couplings with a central metal ion (*e.g.*, Cu^{2+}), the extension of this approach involves an additional sum over nuclear spin projections of that nucleus. This occasional complication becomes increasingly unimportant as the microwave frequency is increased.

We emphasize that the essence of this approach is the conceptual one of defining the orientation subset associated with each ENDOR spectrum and tracking it across the EPR envelope, but also stress the computational advantage, that a simulation for a spectrum at a particular field involves a single integral over an orientation variable. This may be contrasted with most other approaches which achieve orientation selectivity only while performing a full powder average (double integral over the unit sphere).

Computation

The equations underlying this strategy have been implemented in an interactive QUICKBASIC program for PC's; a compiled version is currently available from our website (http://endor1.chem.nwu.edu), along with a 'manual' for the use of the 2-program suite. The program GENDOR simulates polycrystalline ENDOR spectra for an EPR spectrum determined by a g-tensor of arbitrary symmetry (axial or rhombic) without resolved hyperfine structure. The ENDOR under analysis is assumed to be from a nucleus with unresolved hyperfine structure whose tensor (A) is of arbitrary symmetry and orientation with respect to g-frame. The quadrupole tensor (P) for $I \geq 1$ is assumed coaxial with **A**, except for I = 1, where the quadrupole tensor can be of arbitrary orientation. In general, the program employs perturbation equations for ENDOR frequencies, except for I=1 where it uses exact formulas given by Muha.[2]

GENDOR can do multiple spectral simulations, using a variety of parameter settings controlled by the g_{obs} values. In addition, it can perform multi-nuclei (up to four) simulations with options to save individual and sum spectra. Simulated spectra may be centered at the Larmor frequency of each individual nucleus. This feature is particularly useful when one is simulating a set of proton resonances across the EPR envelope and for ENDOR spectra taken at higher microwave frequencies where there is a substantial shift in Larmor frequencies across the EPR envelope. A program ESDIP is used to create the input datafile that is used by GENDOR.

A second-generation program suite, GENSIM, written in C and optimized for speed (see below), is under development and will made available in due course. A 'beta' version can be obtained by direct contact with PED.

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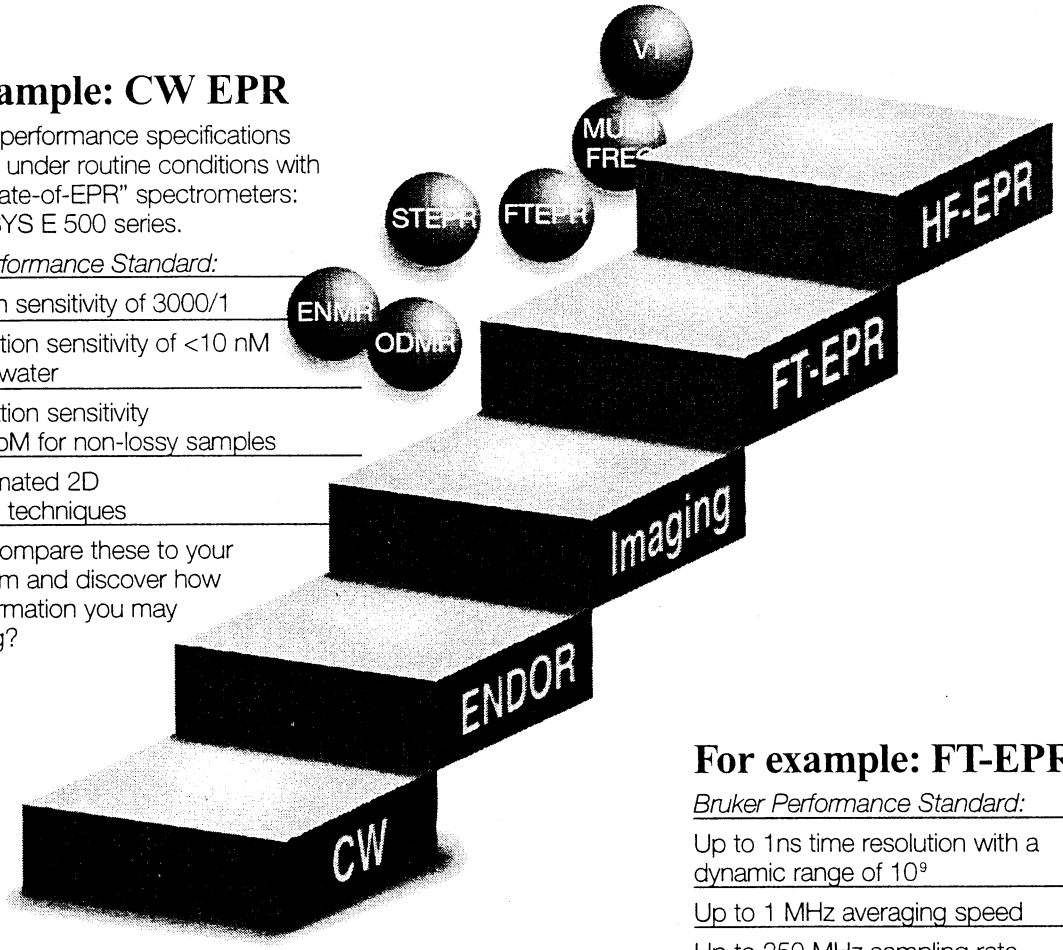

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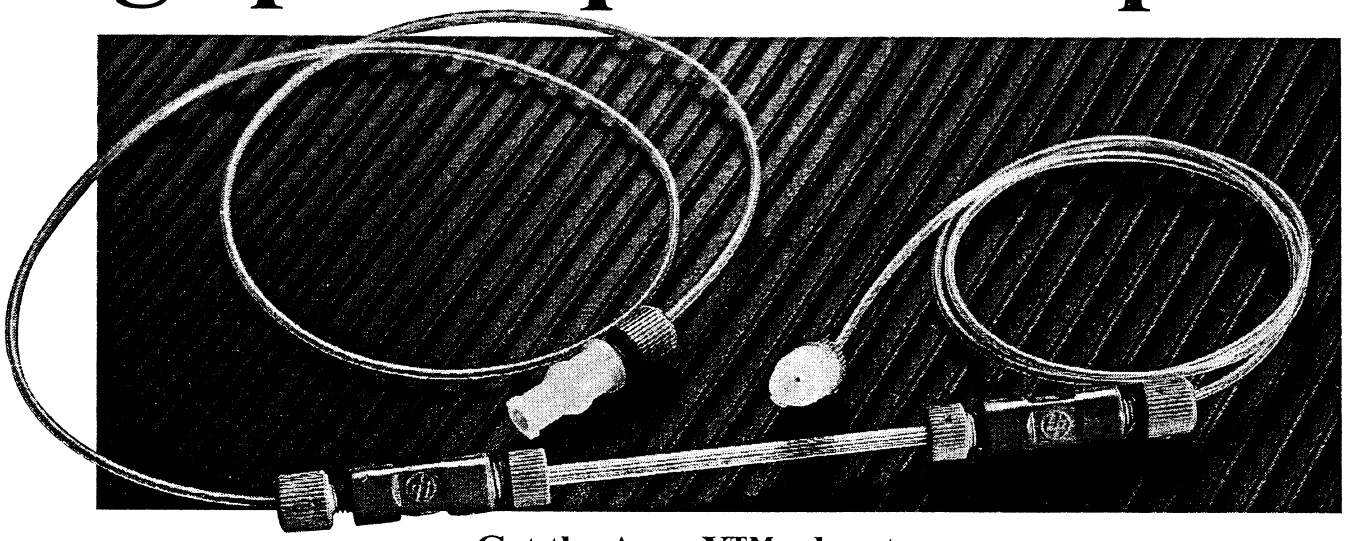

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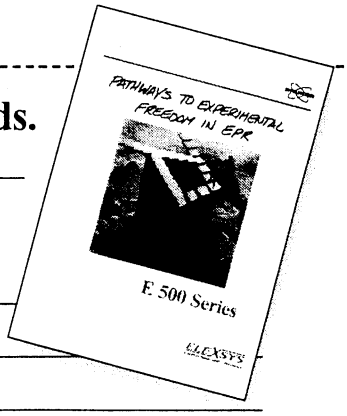

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Outline of Analysis Procedure

The key element of this approach is to examine the full data set for the 2D pattern it displays in the variation of the frequencies and relative intensities of the spectroscopic features with field. As a thumbnail description, the process of obtaining hyperfine tensor principal values and orientations might go as follows. It begins with the accumulation and indexing of ENDOR spectra at multiple fields across the EPR envelope, and by noting the maximum coupling (A_{max}) and the field at which it occurs. Next, a first approximation to the hyperfine principal values A_3 and A_1 is obtained from the ENDOR frequencies measured in the single-crystal-like spectra obtained, respectively, at the high- and low-field edges of the EPR envelope; A_2 is estimated from the spread of frequencies (when observable) in the spectrum taken at $g_{mid} = g_2$. Then, the nature of the relative orientation of the **g** and A tensors is inferred from the development of the ENDOR pattern as the field increases from the low-field, g_1, and/or high-field, g_3 edges of the EPR spectrum; note the requirement that one of the principal values must correspond to A_{max}. At this stage, numerous simulations of selected spectra typically are performed by varying the hyperfine principal values and the relative orientation of g-tensor and nuclear coordinate frames. The analysis begins with the simplest assumption, namely the minimal noncoaxiality of g and A tensors and is terminated when the entire (accessible) field-frequency pattern of ENDOR features had been accommodated. To recreate the 2-D pattern, the ENDOR linewidths is set as the width of the narrowest observed feature, while the possible influence of a non-zero component EPR linewidth is ignored. The final step, to accurately simulate the individual spectra, requires consideration of the effects of the EPR linewidth, which introduces differential broadening that can influence the appearance and even positions of some ENDOR features. The program GENDOR is satisfactory in speed up to this point; the enhanced speed of the new programs GENSIM makes them superior with non-zero EPR linewidth.

For systems with resolved ENDOR splittings from a nucleus with $I > ½$, it is possible to use these procedures to determine quadrupole and hyperfine tensors simultaneously.

Selected References:

(*1*) Hoffman, B. M.; Martinsen, J.; Venters, R. A. *J. Magn. Reson.* **1984**, *59*, 110-123.

(*2*) Hoffman, B. M.; DeRose, V. J.; Doan, P. E.; Gurbiel, R. J.; Houseman, A. L. P.; Telser, J., *in* "Biol. Magn. Reson."; Vol. **13**, (Berliner, L. J. and Reuben, J., Eds), pp. 151-218, Plenum Press, New York and London (1993).

(*3*) Sturgeon, B. E.; Burdi, D.; Chen, S.; Huynh, B.-H.; Edmondson, D. E.; Stubbe, J.; Hoffman, B. M. *J. Am. Chem. Soc.* **1996**, *118*, 1551-7557.

(*4*) Willems, J.-P.; Burdi, D.; Lee, H.-I.; Doan, P. E.; Stubbe, J.; Hoffman, B. M. *J. Am. Chem. Soc.* **1997**, 9816-9824.

(*5*) Lee, H.-I.; Dexter, A. F.; Fann, Y.-C.; Lakner, F. J.; Hager, L. P.; Hoffman, B. M. *J. Am. Chem. Soc.* **1997**, *119*, 4059-4069.

(*6*) Lee, H.-I.; Doan, P. E.; Hoffman, B. M. *J. Magn. Reson.* **1999**, *140*, 91-107.

Building the Perfect Beast

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ELECTRIC DISCHARGE MACHINING - EDM

Many of the microwave component designs that are commonly used in electron magnetic resonance tend to be difficult to fabricate by conventional machining methods. For example, the Mims transmission line sample resonator consists of an H-shaped well that is made in a brass block, and the dimensions of this lower piece, which acts as a shunt to a pair of parallel rectangular guide section, must closely match the apertures in the waveguide. A second complication is the taper sections that are used to match the ½ filter section (the brass block, assembled) and the standard waveguide. The original probehead of Mims made at Bell Labs looked like something handed down by the gods; most machinists noticeably blanch at the sight of it because of the blind cuts and small radii between walls that cannot be reproduced by standard milling methods.

I eventually found out that the probehead was manufactured by an EDM technique, which is an electrochemical process run amok. A workpiece and electrode are brought into close proximity in a bath of dielectric fluid. The two pieces are biased by a high voltage in such a way that an electrical arc is set up across the two 'electrodes'. Depending on what book you read, the workpiece is cut (I would call it fine-controlled pitting) by metal 'melting' via the heat of the electrical discharge or a vastly accelerated electrochemical process (e.g. Cu(O) - Cu(+n)) because of the overvoltage. The dielectric (often kerosene, but because of soot production alternate dielectric fluids are recommended) is usually continuously flushed over the workpiece/electrode combination. The quality of the cut varies with the magnitude of the spark, which should depend on such factors as the distance between workpiece and electrode, the dielectric fluid, and the applied voltage.

There were several articles in *The Home Shop Machinist* that describe EDM process and give sketchy plans on how to build a small EDM apparatus. Basically, these things consist

of a low-tech power supply similar to the ones that you find in these beginner books on electronics (there is a pretty good one published by Radio Shack, for example), except that the thing is going to pull several amps at 60 Vdc. Langlois' "Part 2" in the series describes the construction of a spark power supply in detail.

The actual power supply requirements are going to depend upon the nature of the cut. For example, a Mims cavity is going to require a spark discharge from an electrode approaching the dimensions of a WR-90 waveguide, and the current will obviously be commensurate with the electrode area. The machining process itself is effected by mounting the electrode in such a fashion that it may be moved linearly (as on a drill press) which for most simple cases entails a stepper motor. The cuts are 'cleaner' when one keeps the sparks small, and at least one design for the home shop that I have seen mounts the electrode on a vibrating scriber (one of the Dremel tools) in order to improve the uniformity of the cut. The latter apparently obviates the problem of setting up a standing arc and pitting; the idea is analogous to keeping the working electrode surface clear of adsorbed layers in electrosynthesis.

ONE FINAL NOTE: A recent issue of NASA Tech Briefs (Vol. 21, no. 9, p78) describes a wire EDM setup that enables one to work large pieces along multiple planes. The thing resembles an XY-recorder mounted on its end and on a linear translation stage. As for our own fabrication of probehead, I ultimately decided to do the actual opposite of EDM: I had the Mims probehead sections fabricated via the electroform method, which lays down a metal 'shell' onto an electrode. The mandrel is then either slid away from the formed piece or dissolved, depending on the material and complexity of the design. The mandrel/electrode on which the metal layer is deposited can be precisely machined, and one obtains well-fitting junctions whose tolerances are set only by those of the machined mandrel, which are usually much better than milling. This approach proved very cost effective (approximately $350 for a 0.05" wall piece without flanges, such as a 12" Gordon Coupler section or a Mims cavity 'shell') and yielded components that on assembly were characterized by much lower VSWR than both the Mims EDM unit (in part, because I was able to eliminate one waveguide junction by going with electroform) and similar profiles made by brazing brass wedges into standard rectangular guide.

References:

- Amsbury, C.R., "A Spark Erosion Machine," *Model Engineer,* 1976 July, 688.
- Langlois, R.P., "Electrical Discharge Machining - Removing Metal by Spark Erosion, Part 1," *The Home Shop Machinist,* 1995 (3), p22.
- Langlois, R.P., "Electrical Discharge Machining - Removing Metal by Spark Erosion, Part 2," *The Home Shop Machinist,* 1995 (4), p40.
- Langlois, R.P., "Electrical Discharge Machining - Removing Metal by Spark Erosion, Part 3," *The Home Shop Machinist,* 1995 (5), p34.

- Meador, H., "Electric Discharge Machining," *The Home Shop Machinist, 1991 (1),* p.42.
- Meador, H., "Electric Discharge Machining," *The Home Shop Machinist, 1991* (4), p.4.
- Meador, H., "Electric Discharge Machining," *The Home Shop Machinist,* 1994 (3), p.44.
- Washburn, R.A., Root, L., "A Shop-Made, Shop-Size Electric Discharge Machine," Strictly IC, 1993 Aug/Sept., p.3
- Washburn, R.A., Root, L., "A Shop-Made, Shop-Size Electric Discharge Machine," Strictly IC, 1993 Oct/Nov. p.3.
- Washburn, R.A., Root, L., "A Shop-Made, Shop-Size Electric Discharge Machine," Strictly IC, 1993 Dec/Jan, p3.

TIPS & TECHNIQUES

Single-Axis Crystal Holder for EPR Work, and Use of Powdered DPPH as a g-Standard

Ning Chen, Yuanming Pan and John A. Weil
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University of Saskatchewan, Saskatoon, SK Canada

Concentrated 2,2-diphenyl-1-picrylhydrazyl (DPPH) is a frequently useful standard for $g = h\nu/\beta_e B$ since this material is chemically quite stable and has a narrow powder linewidth (ca. $\Delta B = 1.9$ G for the max-min field spacing of the X-band first-derivative presentation). The powder lineshape is not far from being a single lorentzian line. The signal is not normally (say, for < 100 mW) subject to appreciable power saturation. The g factor in our sample in air, as measured at the zero (cross-over) position, is 2.00354. This value was determined by using an evacuated dilute benzene solution (0. 1 mM) of DPPH, which has g = 2.003 54 [1]. This calibration was done since it is known that the EPR parameters depend to some extent on the preparation details (e.g., solvents used) and previous history of the sample, and mildly on any dioxygen present.

The exchange-narrowed single line is so intense for any sample consisting of more than a speck or two of DPPH that it is likely to swamp the signal of the actual sample S being

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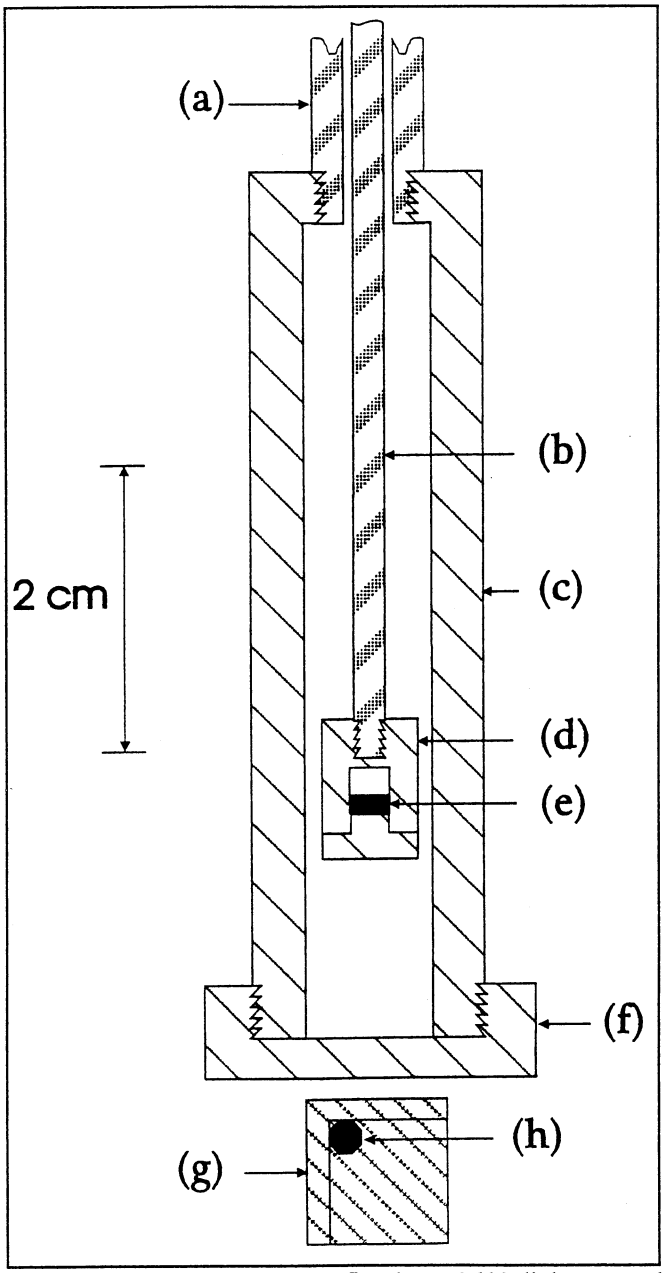
studied, so that one is induced to minimize the quantity of DPPH used, leading to a minuscule sample. However, since crystals of DPPH show appreciable g anisotropy ($0 \leq \Delta g \leq 0.001$ [2]), as well as of the linewidth, it is not safe to use only a speck or two when doing single-crystal work, i.e., when rotating a crystal S relative to the field **B**.

In this situation, we have found it expedient to continue working with a large sample of DPPH, but using the sample holder depicted in Figure 1 consisting of the following components:



1. Threaded brass tube (a) fitted to a 360° dial mounted well above (ca. 20 cm) the resonator. A Bruker wide-bore X-band cylindrical resonator 4107WZ was utilized in our work.

2. The brass tube holds a slip-fit brass rod (b) and is designed to hold a cylindrical virgin teflon jacket (c), screwed onto the bottom end of the tube and hollowed to contain a two-piece teflon DPPH sample holder (d) screwed to the bottom of the rod. The rod, holder and DPPH sample (e) are movable up and down, and the length of the rod extruding from the top of the tube allows measurement of this sample's position relative to the resonator.

3. Teflon bottom plate (f), screwed onto cylinder (c), with flat bottom.

4. Acrylic hollowed-out three-sided cube (g), with side length 0.6 cm, used to hold the sample S (h). This is attached to part (f) with heavy silicone grease. It is detachable to enable reorienting it as well as separate x-ray diffraction measurement used to determine the orientation and to align the crystal S within the cube.

Thus we have solved the above DPPH sample problem by using a fairly massive sample (ca. 0.2 mg) of the powder, guaranteeing adequate orientational averaging of its many crystallites, but placing it almost out of the cavity so as to obtain only a suitably small signal (or none). Thereby the DPPH sample now acts as completely isotropic. The figure shows its (adjustable) position in the cylindrical sample holder. Of course, a calibration must be made to correct for any difference in magnetic field between the location of the DPPH and sample S (ca. 1 G in our case).

The accurately machined plastic cube holding the crystal S allows one to carry out three orthogonal rotations of that crystal[3], merely by attaching it to the flat plate on each of its three faces, in turn. In our case, S was an apatite crystal doped with ca. 1% by weight of Gd(3+). Not shown is an attachable Al template which serves to set the orientational position of the cube relative to the teflon cylinder and goniometer when attaching the cube.

REFERENCES:

[1] J. A. Weil, J. R. Bolton and J. E. Wertz, *Electron Paramagnetic Resonance - Elementary Theory and Practical Applications,* John Wiley & Sons, New York, NY, USA 1994. Page 511.

[2] Yu. V. Yablokov, Doklady Akademii SSSR (Engl. Transl.) **133**, 424-426 (1960).

[3] The number of rotations required depends on the crystal symmetry. See: J.A. Weil, T. Buch and J.E. Clapp, Adv. Magn. Reson. **6**, 183-257 (1973), Table V.

BOOKS & PROCEEDINGS

Joint VI International Workshop Electron Magnetic Resonance of Disordered Systems and IV International Seminar on Applied EPR, June 7-14, 1998, Sofia, Bulgaria

Both biannual meetings were organized by the Bulgarian EPR Society in collaboration with Institute of Catalysis, Bulgarian Academy of Sciences and Department of Chemistry, Sofia University.

Representatives from 16 countries (Austria, Belgium, Croatia, Denmark, France, Germany, Israel, Italy, Japan, Poland, Russia, Saudi Arabia, Slovak Republic, Switzerland and Bulgaria) attended both meetings.

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

a. **EMARDIS:** •M. Brustolon, *Dephasing of electron spin echoes: Spin dynamics of the matrix or spatial dynamics of the probe?*; •L. Duelund, *EPR characteristics of some non-heme low-spin iron(III) complexes*; •S.A. Dzuba, *Amplitudes of libration motion of guest spin probe molecules in organic glasses*; •G. Grampp, *Solvent dependence of electron transfer reactions: Recent experimental results and theoretical developments*; •J.S. Hwang, *Frequency dependent study of the correlation functions in EPR spectroscopy – the Cole-Davidson approach*; •Y. Ohba, *Some advantages of fast linear prediction in analysis of time domain magnetic resonance signals*; •C. Oliva, *Ordered structures, spin bags and ferromagnetic domains in spin-like and perovskite-like catalysts, as observed by EPR spectroscopy*; •A. Ponti, *Simulation of magnetic resonance powder spectra: Rigorous assessment and new approaches*; •S. Stoll, *Pulsed EPR investigations of axially coordinated Co(II)-heptamethyl corbyrinate, a coenzyme B12 model*; •V.F. Tarasov, *Time-Resolved ESR spectroscopy of spin correlated micelle confined radical pairs. The spectral shape of anti phase structure*; •A.M. Volodin, *Ion radicals as spin probes for investigation of active sites on the surface of oxide catalysts;* •H. Vrielinck, *Magnetic resonance study of Rh complexes in AgCl microcrystals*; •J.-L. Zimmermann, *Metal-phosphate interactions in biological systems probed by ESEEM and HYSCORE*;

b. **APPL-EPR**: •K. Dyrek, *Quantitative EPR as a tool for investigation of surface and bulk properties of oxide catalysts*; •A. Blank, *Quantitative EPR: Numerical calculation of the EPR filling factor*; •T. Herrling, *Nitroxide reduction in human skin - determination of the antioxidative potential*; •A. Jezierski, *EPR studies on stable and transient radicals in humic substances from compost, soil, peat and brown coal*; •K. Jung, *Toxic effects of Cu(II) in bacillus subtilis cultures*; •T. Herrling, *EPR for everybody - MICROspec-X a new class of EPR spectrometer*; •B. Rakvin, *Study of relaxation rates of stable paramagnetic centers in gamma-irradiated alanine: Influence on alanine/ESR dosimetry*; •G. Vanhaelewyn, *An EPR spectrum decomposition study of irradiated alanine*; •P. Rapta, *In situ ESR and UV-vis spectroelectrochemistry of conducting polymers and supramolecular structures*; •V. Gancheva, *New generation of SS/EPR dosimeters. Physico-technical data of alanine/EPR dosimeters.*

Poster presentations:

a. **EMARDIS:** •G. Grampp, S. Landgraf, S. Strauss, K. Rasmussen, *ESR-linebroadening effects of the DDQ/DDQ$^-$ electron-self exchange couple. Unexpected solvent dependence. (DDQ=1,2-dichloro-4,5-dicyano-p-benzoquinone)*; •St. Stoll, A. Schweiger, *MATLAB toolbox for modelling EPR spectral data*; •G. Sarova, D. Roussanova, B. Jeliazkova, N.D. Yordanov, P. O'Brien, *CT photo-chemistry of bis(diethyldiselenocarbamato)copper(II);* • A.M. Volodin, *In situ ESR study of the state of Fe ions in FeZSM-5 zeolites.*

b. **APPL-EPR**: •N.D. Yordanov, V. Gancheva, S. Ivanova, J. Raffi, S. Chabane, L. Douifi, *EPR and TL detection of irradiated agricultural products*; •N.D. Yordanov, V. Gancheva, J. Empis, A. Lund, W. Stachowicz, G. Vanhaelewyn, *Self-calibrated alanine/EPR dosimeter. Results from the International intercomparison trial;* •N.D. Yordanov, S. Lubenova, *Dependence of absolute and relative to reference standard EPR response on sample containers diameter, dielectric properties of the sample and modulation frequencies;* •N. D. Yordanov, S. Lubenova, *Selective estimations of NO_2 in air, NO_2^- and NO_3^- in vegetables and fruits by the EPR spectrometry*; •N.D. Yordanov, S. Lubenova, *Separate determination of pyrolyzed products (soot and polycyclic aromatic hydrocarbons) in air by EPR spectrometry.*

Two Round Table Discussions were organized: "EMR at the frontier of XXI century" (moderators M. Brustolon, N.D. Yordanov) and "APPL-EPR in the XXI century" (moderators K. Dyrek, A. Jezierski, N.D. Yordanov).

The full text of all presented lectures as well as selections from the short original communications will be published as a special issue of *Spectrochimica Acta, Part (A)* in the beginning of 2000.

Following the established tradition for easy scientific contacts and discussions on the individual level the number of the participants was limited to about 30 persons. All of them were accommodated in a small hotel, situated in the Vitosha mountains, about 10 km away from downtown Sofia, in which all meals were taken. Lectures presentation and free evening discussions were held also in the same place.

Social programme included cocktail, farewell dinner in a traditional Bulgarian restaurant, one-day excursion to the Rila Monastery and half-day sightseeing tour in Sofia .

The next meetings of these series are scheduled to be held during the first year of the next century.

Address for correspondence: N.D. Yordanov (Convener), V. Gancheva (Sci. Secretary), Inst. Catalysis, Bulgarian Acad. Sciences, 1113 Sofia, Bulgaria. ☎: (+3592) 979-2546 or 724-917; FAX: (+3592) 756-116. E-mail: ndyepr@bas.bg or ndyepr@ic.bas.bg.

NOTICES of MEETINGS

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

INTERNATIONAL SOCIETY for MAGNETIC RESONANCE in MEDICINE 8th SCIENTIFIC MEETING and EXHIBITION, Denver, Colorado, April 1-7, 2000.

The Eighth Scientific Meeting of the International Society for Magnetic Resonance in Medicine will take place 1-7 April 2000 at the Colorado Convention Center in Denver, Colorado, USA.For full details, please contact the ISMRM office, ☎: 1-510-841-1899, e-mail: info@ismrm.org; or visit the Society's web page:

http://www.ismrm.org/

HIGH-FREQUENCY ELECTRON PARAMAGNETIC RESONANCE: TECHNOLOGY and APPLICATIONS, Amsterdam, The Netherlands, April 12-14, 2000.

This conference is being organized under the auspices of the Academy Committee for Chemistry of the Royal Netherlands Academy of Arts and Sciences. The local organizing committee consists of Peter Gast, Edgar Groenen, Arnold Hoff, and Jan Schmidt. The aim of the conference is to report on the progress in the technology of High-Frequency EPR and on applications in physics, chemistry and biology. The program will consist of invited and contributed lectures and poster presentations. A brochure was sent to IES members with the previous EPR Newsletter (v.10, #2). Scientists interested in contributing to or participating in this conference are invited to contact the web page:

http://www.knaw.nl/hfepr

For further information contact Mr. R. des Bouvrie, Royal Netherlands Academy of Arts and Sciences, P.O. Box 19121, 1000 GC Amsterdam, The Netherlands; E-mail: roy.des.bouvrie@bureau.knaw.nl; ☎: 31-20-55-10-730; FAX: 31-20-62-04-941.

3rd WORKSHOP ON EPR INSTRUMENTATION AND METHODOLOGY, National Biomedical EPR Center Biophysics Research Institute, Medical College of Wisconsin, Milwaukee, Wisconsin, May 5-6, 2000.

Our Third Workshop on EPR instrumentation and methodology will be held Friday and Saturday, May 5 and 6, 2000. The title of this workshop is "EPR Methods in Structural Biology." The first day will consist of lectures, while the second day will be devoted to hands-on demonstrations, discussions, and tours of the National Biomedical EPR Center.

This workshop is supported by the National Center for Research Resources of the National Institutes of Health. The workshop will mark the 25th year of funding for the National Biomedical EPR Center by NCRR.

The budget for the workshop is limited, but it is expected that a portion of the living expenses while attending the Conference will be covered. Also, a limited number of travel awards for students may be available.

If you are interested in attending, please contact Christopher C. Felix, Ph.D., Scientific Administrator, 8701 Watertown Plank Road, P.O. Box 26509, Milwaukee, WI 53226-0509, USA; ☎: 414-456-4000, Fax: 414-456-6512, E-mail: cfelix@mcw.edu

42nd Rocky Mountain Conference on Analytical Chemistry; 23rd INTERNATIONAL EPR SYMPOSIUM, Broomfield, Colorado, July 30-August 3, 2000.

Sponsored by the Rocky Mountain Section Society for Applied Spectroscopy and the American Chemical Society Colorado Section. Major Symposia on EPR and NMR are held at this conference. Details will be published in future editions of this newsletter, or visit the following web site:

http://www.milestoneshows.com/events.html

XIXth INTERNATIONAL CONFERENCE on MAGNETIC RESONANCE in BIOLOGICAL SYSTEMS (XIX ICMRBS), Florence, Italy, August 20-25, 2000.

You are cordially invited to attend the XIXth International Conference on Magnetic Resonance in Biological Systems (XIX ICMRBS) to be held in Florence, Italy from August 20 to 25, 2000. Florence is easily accessible both by train (ca. 1.5 hrs from Rome by fast train) and by plane. The airport, located 5 Km from the city center, is connected, through direct flights, with the major Italian and European cities.

Scientific Program–The scientific program will cover a wide range of research topics in the field of magnetic resonance applied to biological systems. Particular attention will be devoted to new and promising areas of research as well as to emergent methodological tools within the frame of NMR research in the post-genomic era. The scientific agenda will include plenary lectures, session lectures and poster presentations. The sessions will be organized on the following topics: protein structure, folding, and mobility; EPR/ENDOR applications; membrane proteins; In vivo spectroscopy and imaging; DNA, RNA, nucleotides and their interaction with proteins; SAR of drugs and drug discovery; computation and dynamics.

Location–The conference will take place at the Centro Internazionale Congressi and Palaffari Firenze located close to the central railway station in the historical and monumental area of Florence.

Accommodation–Accommodation will be arranged in hotels of different categories, mostly within walking distances from the venue (student dorms will be available). Detailed information and reservation forms for accommodation will be included in the second circular.

Change of Address–Information on the scientific program, accommodation, general arrangements, registration forms and instructions for preparation of abstracts are continuously updated in our web site. Please visit it! Registration can be done on line. Abstract and early registration deadline is March 31, 2000. For further information, please contact the XIX ICMRBS Secretariat, Dept. Chemistry & CERM, Univ. Florence, Via Luigi Sacconi 6, I-50019 Florence, Italy; ☎: 39-055-4209260; Fax: 39-055-4209253; E-mail: icmrbs@cerm.unifi.it. Or visit the web address at:

http://www.cerm.unifi.cnr.it//icmrbs.html

Conference Committees: *Organizers:* I. Bertini, (Florence, Italy) Chairperson; L. Banci (Florence, Italy) Ex. Manager; R. Kaptein (Utrecht, The Netherlands); H. Rueterjans (Frankfurt, Germany); G. Valensin (Siena, Italy). *Assistants to the organizers*: R. Del Conte & I.C. Felli (Florence, Italy); Treasurer: P. Turano (Florence, Italy). International Advisory Board: A.S. Arseniev (Moscow, Russia); C.M. Dobson (Oxford, U.K.); S. Forsen (Lund, Sweden); G. Govil (Bombay, India); A.M. Gronenborn (Bethesda, USA); C.W. Hilbers (Nijmegen, The Netherlands); J.S. Hyde (Milwaukee, USA); C. Ho (Pittsburgh, USA); M. Kainosho (Tokyo, Japan); J.F. Lefevre (Strasbourg, France); J.L. Markley (Madison, USA); A. McDermott (New York, USA); K. Möbius (Berlin, Germany); R.S. Norton (Parkville, Australia); S.J. Opella (Philadelphia, USA); M. Rico (Madrid, Spain); J. Seelig(Basel, Switzerland); B.D. Sykes (Edmonton, Canada); W. Tang (Nanjing, China); G. Varani (Cambridge, U.K.); A. Walker (Tucson, USA). *National Organizing Committee*: Coordinator: A. Rosato (Florence, Italy); S. Aime (Torino); R. Basosi (Siena); R. Bazzo (IRBM); F. Conti (Roma); A. Di Nola (Roma); A. Lai (Cagliari); S. Mammi (Padova); B. Maravigila (Roma); C. Marchioro (Glaxo); G. Martini (Firenze); H. Molinari (Verona); V. Pavone (Napoli); A. Perico (CNR, Italy); F. Podo (Ist. Sup. Sanita); A. Rigo (Padova); A.L. Segre (CNR); A. Spisni (Parma); M. Tato' (Pharm.& Upjohn); P.A. Temussi (Napoli); A. Tomasi (Modena); A. Tramontano (IRBM); F. Uggeri (Bracco); L. Zetta (CNR). *Chairperson of Local Organizing Committee:* R. Pierattelli (Florence, Italy).

6TH INTERNATIONAL SYMPOSIUM on SPIN TRAPPING: "SPIN TRAPS, NITROXIDES and NITRIC OXIDE SPECTROSCOPY, CHEMISTRY and FREE RADICAL BIOLOGY, Marseille, France, August 27-31, 2000.

Tentative Topics–The Scientific Committee has selected a broad range of topics: •Synthesis of novel nitroxides; •Synthesis of novel nitrones and nitroso spin traps; •Synthesis of nitric oxide and peroxynitrite donors; •Nitric oxide and peroxynitrite traps; •Spin trapping of superoxide and nitric oxide derived from nitric oxide synthases; •*In vivo* trapping of nitric oxide; •Pharmacokinetics of spin traps and spin adducts, bioreduction of nitroxides; •Nitroso hemoglobin; •Nitrone traps: antagonists of neuronal injury, ALS, and neurodegenerative diseases; •Chemistry and biology of nitroxyl anion.

Location–It is a great honour that Marseille has been chosen as the conference site. Marseille has a reputation for hospitality towards people from all nations. Its geographic location and ready accessibility offers a convenient and pleasant setting to host an international meeting.

We hope to match the excellence of the scientific sessions with an enjoyable and memorable social programme. We look forward to seeing you in Marseille in the year 2000.

Scientific Committee: A. Alberti *(Univ. Bologna, Italy)*; O. Augusto *(Univ. São Paulo, Brazil)*; M. Davies *(Heart Research Inst. at Sydney, Australia)*; B.C. Gilbert *(Univ. York, UK)*; L. Greci *(Univ. Ancona, Italy)*; K.U. Ingold *(Natl. Research Council at Ottawa, Canada)*; B. Kalyanaraman *(Medical Coll. Wisconsin, USA)*; K. Makino *(Univ. Kyoto, Japan)*; R.P. Mason *(NIEHS, USA)*; A. Rassat *(Ecole Normale Supérieure, Paris, France)*; A. Tomasi *(Univ. Modena, Italy)*; P. Tordo *(Univ. Provence, Marseille, France)*; J.L. Zweier *(Johns Hopkins Medical Inst., Baltimore, USA)*.

Local Organization: Prof. Paul Tordo and the memberships of *VMR 6517 "Chimie, Biologie et Radicaux Libres"* (association CNRS and Aix-Marseille 1 & 3 Universities).

Congress Secretariat: Atout Organisation Science, 6th International Symposium on Spin Trapping, 106 Corniche Kennedy, 13007 Marseille, France; ☎: 33-0-4-91-52-75-10; FAX: 33-0-4-91-52-93-73; E-mail: atoutsci@atout-org.com; or, for full meeting information visit the Congress web-site:

www.up.univ-mrs.fr/~wsrep/spin.trapping.meeting.html

AMPÉRE SUMMER SCHOOL on "APPLICATIONS of MAGNETIC RESONANCE in NOVEL MATERIALS," Nafplion, Peloponese-Greece, September 3-9, 2000.

The Ampére Summer School on "Applications of Magnetic Resonance in Novel Materials" will be held at Nafplion (Peloponese-Greece) 3-9 September 2000. The scope of the School is to introduce magnetic resonance techniques and their use in the investigation of current topics of Materials Science: 1) Disordered Systems and Glassy Materials; 2) Liquid Crystals; 3) Modulated and Incommensurate Systems; 4) Novel Electronic Conductors; 5) Ferromagnetic and Paramagnetic Systems; 6) Porous Systems; 7) Imaging of Materials; and 8) Bio-materials. Apart from NMR and MRI techniques, EPR and Mossbauer Spectroscopy will be also introduced.

The scientific program includes invited plenary lectures, oral and poster contributions. Young scientists are strongly encouraged to participate in the school and present their research activities in oral and poster contributions. The

following lecturers will present one-hour plenary lectures: •Prof. Jersy S. Blicharsky *(Krakow, Poland)*; •Prof. Robert Blinc *(Ljubljana, Slovenia)*; •Prof. Bernhard Blumich *(Aachen, Germany)*; •Prof. Ferdinando Borsa *(Ames, Iowa)*; •Prof. Detlef Brinkman *(Zürich, Switzerland)*; •Prof. H. J. M. De Groot *(Leiden, Netherlands)*; •Dr. Jannis Deligiannakis *(Athens, Greece)*; •Prof. Jani Dolinsek *(Ljubljana, Slovenia)*; •Prof. Franz Fujara *(Dortmund, Germany)*; •Dr. Jorge Luis Gavilano *(Zürich, Switzerland)*; •Prof. Clare Gray *(NY, USA)* -not yet confirmed; •Prof. Mladen Horvatic *(Grenoble, France)*; •Prof. Kazushi Kanoda *(Tokyo)*-not yet confirmed; •Prof. Raymond Kind *(Zürich, Switzerland)*; •Prof. Serge Lacelle *(Quebec, Canada)*; •Prof. Fanny Milia *(Athens, Greece)*; •Prof. Pierre Panissod *(Strasbourg, France)*-not yet confirmed; •Prof. Moshe Paz-Pasternak *(Tel Aviv, Israel)*; •Prof. Vasilis Papaefthymiou *(Ioannina, Greece)*; •Dr. Josef Roos *(Zürich, Switzerland)*; •Dr. Josef D. Seymour *(Albuquerque, USA)*; •Prof. Jan Stankowski *(Poznan, Poland)*; •Prof. Josef Zwanziger *(Indiana, USA)*.

The School will be held at XENIAS PALLAS hotel, which rises above the town of Nafplion, at the southern coast, and is built in the middle-age castle of Akronafplia. Social and cultural events, as well as an official dinner will be arranged for the participants and the accompanying persons. For on-line registration and more information about the summer school and the town of Nafplion, please visit the web site of the Summer School at:

www.ims.demokritos.gr/nmrlab/conference/

For more information, please E-mail G. Papavassiliou at gpapav@ims.demokritos.gr

POSITIONS AVAILABLE & WANTED

TENURE-TRACK POSITION AVAILABLE at ILLINOIS STATE UNIVERSITY

The following is an ad for a position in a new program at Illinois State University. Although this ad is written for an Assistant Professor position, the committee will accept applications from persons with existing research programs who can "hit the ground running." Excellence in research and teaching which will further the BMB program are the goals for the person who will fill this position.

Tenure-track Assistant Professor to contribute to the new Biochemistry and Molecular Biology (BMB) B.S. program administered by the Departments of Biological Sciences and Chemistry. Preferred starting date: August 16, 2000. The BMB program will prepare students for the revolution in biochemistry, molecular and cellular biology, and biotechnology. The successful applicant will be expected to develop an independent, high quality, and extramurally funded research program, and contribute to training of Ph.D. and M.S. students. Teaching responsibilities will include undergraduate and graduate courses in biochemistry and/or molecular biology. Ph.D. required, postdoctoral experience preferred. To assure full consideration, applications should consist of a CV, copies of 3 publications, 3 recommendation letters and brief statements of research and teaching goals by December 7, 1999. Apply to BMB Search Committee Chair, Campus Box 4100, Illinois State University, Normal, IL 61790-4100. Illinois State University is an equal opportunity/affirmative action employer.

TWO POST-DOCTORAL POSITIONS OPEN at CORNELL

I currently have two openings for postdoctoral associates in my research group. The areas of research will include: 1) Biophysical Studies of Model and Biological Membranes and Dynamic Structure of Membrane Proteins by Modern ESR; 2) Far-Infrared ESR Studies of Molecular Dynamics in Liquid Crystals, Polymers, and Biological Systems; 3) Two-Dimensional Pulsed ESR Studies of Molecular Dynamics in Liquid Crystals, Polymers, and Biological Systems. Interested individuals should contact: Professor Jack H. Freed; B52 Baker Laboratory of Chemistry & Chemical Biology; Cornell University, Ithaca, NY 14853-1301; e-mail: jhf@msc.cornell.edu. Applicants should be prepared to furnish a complete CV and at least two letters of recommendation.

EQUIPMENT & SUPPLIES EXCHANGE

FOR SALE: VARIAN E12 SPECTROMETER

We have a Varian E12 spectrometer, of which the manual part is in good working order, which we would sell for a very nominal price. Enquiries can be directed to: Brain Hasinoff, Univ. Manitoba, Faculty of Pharmacy, Winnipeg, Manitoba, ☎: 1-204-474-8325; FAX: 1-204-474-7617; E-mail: b_hasinoff@umanitoba.ca

FOR SALE: VARIAN E-102 X-BAND BRIDGE

Varian E-102 X-band microwave bridge, with reference arm, fully checked and refurbished, recently replaced klystron with weak pitch S/N test included. Minimum price: US$5,000. To make an offer, contact Vanni Piccinotti, NMR Technical Services, Via del Berignolo 5, 50141 Firenze, Italy. ☎/FAX: 39-055-434841; e-mail: vpnmr@ats.it.

EPR INSTRUMENT WANTED

Searching for an EPR instrument in good working condition with variable temperature attachments. Contact Dr. Horia Caldararu, Romanian Academy, Institute of Physical Chemistry "I.G. Murgulescu," 77208 Bucharest, Romania, FAX: 40-1-3121147; E-mail: hcaldararu@chimfiz.icf.ro or hcaldararu@pcnet.pcnet.ro.

WANTED: USED BRUKER or VARIAN MAGNET

We are looking for a used Bruker or Varian magnet (with or without power supply). If you (or someone you know) have one which is sitting there collecting dust, please let me know.

We will be happy to have it for a reasonable price. Please contact Dr. Jim Liu, Univ. New Mexico, College of Pharmacy, 2502 Marble NE, Albuquerque, NM, 87131; ☎: 1-505-272-9546; FAX: 1-505-272-6749; E-mail: jliu@unm.edu.

AVAILABLE: NITROXIDE RADICALS

A small collection of fairly well-preserved unique nitroxide radicals synthesized by Dr. L.A. Myshkina in the 1980's is now being made available:

- 2,6-bis(N-oxylo-tetramethyltetrahydropyrid-4-yl) thyophene
- 5-(N-oxylo-tetramethyltetrahydropyrid-4-yl) thyophene-2-al
- 2,6-dimethylenecyclohexanone substituted by 6-(N-oxylo-tetramethyltetrahydropyrid-4-yl) thyen-2-yl residues at both alpha-carbon atoms
- 4-chloro-4-nitro-TMP-N-oxyl

Small quantities of the following compounds are also available:

- 4-bromo-4-nitro-TMP-N-oxyl
- 1,4-di-TMP-butaine-bis-N-oxyl

For information about obtaining any of the above compounds, contact: A.E. Myshkin, Inst. Biochem. Phys., Russian Acad. Sci., Kosygin St. 4, 117977 Moscow V-344, Russia; E-mail: chembio@glas.apc.org.

FOR SALE: BRUKER ESP-300 RADIO-SPECTROMETER

The instrument is intended for investigation of materials by means of electronic paramagnetic resonance (EPR). It was purchased from Bruker Analytische Messtechnik GMBH by St. Peterburg quartz-glass factory "Stekvar" in 1989 and was installed in 1990 (tested in April 1990). But it was not used at all, because since that time this research activity was stoped at "Stekvar". It was not moved. Now the instrument is working completely. So, the instrument seems like new. This ESP-300 have maximum specification (for example, there is helium low temperature additional device provided by Oxford Instruments). This instrument is provided with system for double and triple resonance. There are some spare parts. System # is ZD 698. The instrument's technical details are: 1) it works in X-band (frequency: 9.79 GHz); 2) spare cavities: ER 4111VT, ER 4114 HT, ER 4105 DR; 3) NMR magnetometer is ER 035 M with ESR in cavity probe; 4) microwave bridge is ER 044 MRDH; 5) temperature range from 3.5 K (Oxford Instruments helium low temperature unit); 6) double & triple resonance system. For further information, contact Prof. Roman Eismont, E-mail: empire@peterlink.ru; ☎: 7-812-249-02-95; FAX: 7-812-249-51-14; Regular mail: 6 Shafirovsky Avenue, St. Petersburg 195273 Russia.

AVAILABLE: ISOTOPE-CONTAINING SPIN PROBES

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

FOR SALE - NMR MAGNETOMETER

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

WANTED: TERMINAL/MONITOR

Terminal/monitor for Bruker ECS 106 spectrometer wanted. Contact: Lon B. Knight, Jr., Furman University, Department of Chemistry, Greenville, SC 29613, USA; ☎: 1-864-294-3372; FAX: 1-864-294-3559; E-mail: lon.knight@furman.edu.

FOR SALE: VARIAN

Resonance Instruments has available:

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

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

NEED HELP in DESIGN and CONSTRUCTION of EPR ELECTRONICS?

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

AVAILABLE: TWO IBM 9000 COMPUTERS

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

642-2069. E-mail address is: weber@garnet.berkeley.edu; the web site is:

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

AVAILABLE: USED VARIAN EPR EQUIPMENT

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

2) Varian ENDOR accessory, with Varian ENDOR cavity.

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

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

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

For details, contact James Anderson, Research Specialties, 5629 N. Maplewood, Chicago, IL, 60659, USA; ☎/FAX: 1-773-728-6570.

FOR SALE: SPECTRANOVA TEST EQUIPMENT

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

IES INFORMATION AVAILABLE ON WEB

Since e-mail has become a popular means of communication, having correct e-mail addresses is vital. The directory issue helps, but we receive changes almost every day. To assist in communications among EPR researchers, we have put our list of e-mail addresses on the IES WWW. After several electronic mailings to members in recent months, we have also put a "bad" e-mail address list on the web. Messages to members at these e-mail addresses have been returned to the IES as "undeliverable." Please check this list to see if you can help us with updated information. Also, Please check the Web and tell us if your e-mail address and/or payment information is incorrect. The IES home page is at:

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

From this location, you can follow links to membership applications for individual and corporate members, methods of paying dues, your history of dues payments, e-mail addresses, a list of members with invalid mailing addresses, as well as the *EPR Newsletter* web page. All pages are updated regularly.

If you do not have convenient access to the web, or have a question, contact us at IERC@uiuc.edu.

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INFORMATION on JOINING the IES and PAYING DUES

A full version of the membership application, as well as methods to pay dues to one of our regional treasurers around the world, is on the IES web site (address is at the bottom of the previous column).

Membership categories: Full Member (active in EPR/ESR/FMR), dues US$30; Emeritus Member (emeritus or retired status), dues US$10; Postdoctoral Member (this status may be held up to 3 years), dues US$10; Associate Member, dues US$30; Student Member, dues US$5.

To Pay Dues by Credit Card (Visa or MasterCard only), send the following information: type of card you are paying with, amount you are paying, which year(s) you are paying for, account number, cardholder's name, expiration date, and signature. *(If you are paying for more than one person, please be sure to specify each member's name and correct dues amount for that member.)*

Send this information to:

Dr. Chris Felix, Treasurer of the IES
Medical College of Wisconsin
National Biomedical ESr Center
8701 Watertown Plank Road
Milwaukee, WI 53226 USA
Fax: 1-414-456-6512
E-mail: cfelix@post.its.mcw.edu

In many hard-currency areas, we encounter the problem that payment by individual checks is expensive to us because of international exchange costs. (For instance a check written for US$30 on a German bank would cost the Society $25 to collect in the US.) For this reason, regional treasurers do exist in some areas, and we urge members to pay their subscriptions through them for combined transfer to the Society. If you wish to send money to the USA from another country, you must use a draft or international money order drawn on a US bank. We do have a Eurocheque-paying facility in the UK, which may be used by members in the UK and throughout Western Europe. You will pay a very small fee when the amount of the Eurocheque is debited to your account. See the instructions on the web for further details on paying to the UK Regional Treasurer.

If you are unable to pay dues by credit card, Eurocheques or US dollars, please mail your membership form and a short note of explanation to Chris Felix, Society Treasurer.

If you cannot pay in Eurocheques or US dollars easily and cheaply, please think of forming a local payment collective, as the same transfer charge is levied on ten dollars as on a hundred! Please contact Dr. Felix if you wish to make such an arrangement for a local or regional group.

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Zavoisky Award 1999 Goes to Joan H. van der Waals

The Annual 1999 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy went to Professor Joan H. van der Waals (Leiden) in a ceremony marking his outstanding contribution to the investigation of photo-excited triplet state molecules. The ceremony was preceded by the Eighth Annual Workshop: "Modern Development of Magnetic Resonance" 22-24 September 1999.

The selection of Professor Joan H. van der Waals was made from many nominations solicited from international experts in EPR. The Award Ceremony starting in the afternoon of September 24 was attended by over 200 people, among them were the scientists who had participated in the preceding Workshop. The ceremony was chaired by Professor K. M. Salikhov. He, as the Chairman of the Award Committee, announced the decision of the Zavoisky Award Committee. The presentation was made by the Head of the President's Administration of the Republic of Tatarstan E. S. Gubaidullin. The Vice-Rector of the Kazan State University, Professor N. K. Zamov, the Chairman of the Presidium of the Kazan Scientific Centre of the Russian Academy of Sciences, Professor A. I. Konovalov, and the President of the Tatarstan Academy of Sciences, Professor M. Kh. Khasanov warmly congratulated the laureate. Letters of congratulations from Professor B. Maraviglia, President of the AMPERE Society, Professor J.R. Norris, Jr., President of the International EPR Society, and Professor J. S. Waugh, President of ISMAR, were handed to Professor van der Waals. The laureate gave his Zavoisky Award lecture, in which he discussed problems of electron paramagnetic resonance of triplet states. A concert by a string quartet preceded and followed the ceremony. After a meeting with journalists, the guests visited the museum of history of the Kazan State University. The event was concluded with a Banquet in honor of Professor van der Waals and his outstanding contributions to EPR. During a stay in Kazan, the laureate visited places of historical and cultural interest in Kazan and picturesque sites in the town of Elabuga.

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☆☆☆

From the Editor—

This is the Directory issue, containing names, contact information, and in many cases and indication of scientific interests for approximately 4000 scientists. Members of the Society tell us that they find this Directory very useful, but it is only valuable if the information in it is accurate and up to date. We have no way of knowing about errors in the Directory unless you tell us. Please check over your entry carefully and inform us if any changes should be made. For each member of the International EPR Society, you will find up to 5 codes representing your primary fields of interest. Please note that a new field of interest - High Field/High Frequency EPR - has been added recently. If you would like to modify your designated fields of interest, you may do so from our WWW site or by sending us e-mail.

Linn Belford, Editor

✦*IES AFFAIRS*✦

ANNOUNCEMENTS AND REPORTS FROM THE INTERNATIONAL EPR (ESR) SOCIETY

From the President —

It has come to my attention that in 1999 somewhere between one quarter and one third of members have so far paid subscriptions (dues) for the year. The Society cannot function, cover the costs of the half-time staff member in Urbana and pay for the production of the EPR Newsletter, unless the bulk of members pay their subscriptions every year. We will send reminders in the near future along with the call for year 2000 subscriptions. The Society needs to be able to accumulate funds for worthy initiatives such as scholarship support for graduate students to attend conferences. I urge all members to make their payments for 1999 and 2000 as soon as possible.

John Pilbrow, IES President

IN THIS ISSUE

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IES Award Winners to Date —

The International EPR Society has established awards to recognize outstanding scientific achievements. The award winners through 1999 are as follows:

IES Gold Medal: 1992-George Feher; 1993-James Hyde; 1994-Jack Freed; 1995-Sam Weissman (Chemistry); 1996-Kev Salikhov (Physics & Instrumentation); 1997-Harden M. McConnell (Biology & Medicine); 1998-Arthur Schweiger (Chemistry); 1999-Brian Hoffman.

IES Silver Medals Biology/Medicine: 1994-Hal Swartz; 1995-Lev Blumenfeld; 1996-Ron Mason; 1997-Anatole Vanin; 1998-Ed Janzen; 1999-Jack Peisach.

IES Silver Medals Chemistry: 1994-Keith McLauchlan; 1995-Clyde Hutchison, Jr.; 1996-Klaus Möbius; 1997-Hanns Fischer; 1998-Richard W. Fessenden; 1999-Yuri Tsvetkov.

IES Silver Medals Physics/Instrumentation: 1994-Wojciech Froncisz; 1995-Jan Schmidt; 1996-Johann-Martin Spaeth; 1997-Roger Isaacson; 1998-William B. Mims.

IES Silver Medals Physics/Materials Science: 1999-George Watkins.

Young Investigator Awards: 1994-Devkumar Mustafi (Univ. Chicago); 1995-R. David Britt (Univ. California); 1996-Gunnar Jeschke (Univ. Bonn); 1997-Robert Bittl (Techn. Univ. Berlin); 1998-Alex Smirnov (Univ. Illinois); 1999-Ilya A. Shkrob (Argonne National Lab).

Fellows of the Society are listed on page 1 of this issue.

Deadlines Set for Newsletter Materials

Henceforth there will be firm and fast deadlines for the receipt of materials for each issue of the *EPR Newsletter*. They will be published in every issue of the newsletter and on the *EPR Newsletter* web page. The deadlines for 2000 are:

Volume 11 Number 1: **January 31, 2000**
Volume 11 Number 2: **April 30, 2000**
Volume 11 Number 3: **July 23, 2000**
Volume 11 Number 4: **October 31, 2000**

Publishable items arriving after each of these deadlines will be held over for the next issue.

Nominations Open for the Zavoisky Award 2000

The Zavoisky Award 2000 will be presented at the annual Workshop "Modern Development of Magnetic Resonance" in September 2000 in Kazan where E. K. Zavoisky demonstrated EPR in 1944. This prestigious award is given in recognition of an outstanding contribution to the development of electron paramagnetic resonance. 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: B. Bleaney (Oxford), G. Feher (La Jolla), K. Moebius (Berlin), A. Schweiger (Zurich), Yu. D. Tsvetkov

(Novosibirsk), and the Chairman K. M. Salikhov (Kazan). The selection of the Awardee is made after consultations with the Advisory Award Committee which comprises: K. H. Hausser (Heidelberg), C. A. Hutchison Jr. (Chicago), and Yu. N. Molin (Novosibirsk).

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; Fax: 7-8432-765075. **The deadline for submission of nominations is April 1, 2000.**

THE COMPUTER CORNER

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

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

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

****

Xemr - A General Purpose Electron Magnetic Resonance Software System

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Xemr software runs on Linux based systems (Intel, Alpha, power PC, etc.) and can be used for data acquisition, data manipulation, and EMR spectrum simulation though a graphical user interface. Each of these capabilities are described in more detail below. The data acquisition interface currently supports Varian E-line spectrometers (with gaussmeter and field/frequency lock), Bruker ER200D spectrometers, and the Bruker ESP300 spectrometer (in CW mode). In the Varian system, the gaussmeter is connected to an IEEE-488 bus, signal intensity is read by means of an A/D converter, and the magnetic field is controlled by means of a D/A converter. Currently, IEEE-488 cards which are supported by the Llinux-GPIB package (see the Linux Lab project page: http://www.llp.fu-berlin.de) can be used. The A/D and D/A converter supported in this setup is the Keithley DAS8AO. This will, however, change in future versions of Xemr when low level A/D and D/A interfacing is handled by the COMEDI package (see ftp://stm.lbl.gov/comedi) in which case all A/D and D/A cards supported by COMEDI can be used. The other spectrometers have more complicated hardware but can basically be controlled by means of an IEEE-488 controller, A/D, and D/A interfaces in a similar fashion. The supported measurement modes (where available) are: EPR, ENDOR, TRIPLE general, TRIPLE special, ENDOR, induced EPR, and kinetics mode. The measured spectra can be read/saved from/to disk along with the measurement parameters. Since Linux is a multitasking operating system other operations can be performed while the system is obtaining EPR data. The EMR spectra can reside on multiple pages and can be overlaid, shifted, scaled, etc. so that spectral comparisons can be performed. Spectral manipulation operations include the following: spectral add/subtract, differentiate, integrate (both definite and indefinite integrals), smoothing, Fourier transforms with various windowing functions, spectral convolutions, cross/autocorrelations, cepstral analysis, and RMS difference calculations. Also the usual baseline correction methods (polynomial and spline) are available. The spectra can be printed out by using the Xmgr package which can produce postscript and HPGL output. The latter format can be easily included in your favorite word processor document. The Xemr package also includes the ability to convert from Bruker Aspect and Bruker ESP file formats to the internal format of Xemr. The Xemr internal format can be

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exported into XY-ASCII format easily. Actually, the Xemr internal format is very close to XY-ASCII format.

Xemr can perform EPR and ENDOR spectrum simulation to first order or by using a numerical solution of the full spin Hamiltonian. In both cases no special requirements are set for principal axis systems. The first order simulation can only handle S = ½ with electron Zeeman and hyperfine coupling and is most useful when dealing with organic radicals. The numerical approach is more general and can deal with the following spin Hamiltonian:

$$H = \beta_e H \cdot \left(L + g \cdot S - g_N I\right) + \xi L \cdot S + \sum_{i=1}^{ne}\sum_{j=1}^{ne} S_i \cdot D_{ij} \cdot S_j + \sum_{i=1}^{ne}\sum_{j=1}^{nn} S_i \cdot A_{ij} \cdot I_j + \sum_{i=1}^{nn} I_i \cdot P_i \cdot I_i + H_{oct}(L) + H_{tetr}(L)$$

where L denotes the total orbital angular momentum, S the sum of each S_i , I the sum of each I_i , and the rest of the symbols have their standard meaning. Note that the matrices D and A have the electron-electron and electron-nuclear indices, respectively. The product between L and S above should be currently understood so that the spin-other-orbit interactions are ignored. The rightmost elements of the above Hamiltonian are crystal field operators where oct means octahedral and tetr tetrahedral symmetry. For systems where S>½ one can choose between fictitious spin or normal representation. Additionally one can specify manually or according to the Boltzmann distribution which Eigen-levels are active in the simulation. Finally, the transition moments can be calculated using the Fermi golden rule and the following transition operators:

$$H_1(90°) = g_e\beta_e B_1 S_x - g_n\beta_n B_1 I_x$$
$$H_1(0°) = g_e\beta_e B_1 S_z - g_n\beta_n B_1 I_z$$

The problem with the above approach is that when EPR spectra are recorded by varying the magnetic field, then the spin Hamiltonian would have to be diagonalized separately at every field value. Xemr uses an approximative method where the spin Hamiltonian is diagonalized at given field values and the rest of the points are obtained by linear interpolation. Linear interpolation is used for both transition field value as well as for transition moment. Depending on the required accuracy, the number of points can be chosen suitably. The energy levels and transition moments can be visualized in order to help with proper understanding of the system in question. For the obtained transitions, Lorentz or Gauss line shapes can be introduced by the FFT-algorithm. Note that for the first order simulation the nuclear spin dependent line width alternation is also available. Also for exchange systems Heinzer's and Norris' methods are available.

Both the first order and numerical simulation, including all the line shapes described above, can be fed into a powder integrator which will then yield the corresponding powder spectrum. A number of different powder integrators exist in Xemr: Gauss-Legendre (regular or IGLOO), Gauss-Chebysev (regular or IGLOO), various versions of Simpson rule, linear interpolation with respect to integration angles (regular or IGLOO), cubic spline interpolation with respect to integration angles (regular or IGLOO), and special versions of these for the axial case.

By using the above simulation modes one can least-squares-fit the simulated spectrum to the experimental EPR or ENDOR spectrum by Monte Carlo, Simplex, Marquardt, or Hooke-Jeeves methods. To control the optimization the user can define variables and equivalences specific for each system in question. For some difficult cases, variable limits can also be set. This has been implemented through penalty terms which are included in the object function.

Xemr currently consists of *ca.* 22000 lines of C code. I have been writing it mostly on my spare time and sometimes the code looks like that. Finally, Xemr (and Linux by the way) is distributed under the GNU General Public License which basically means that both source and binary versions are distributed and can be redistributed for free.

For more information on Linux see:

http://www.linux.org or http://www.redhat.com

For more information on Xemr see:

http://epr.chem.jyu.fi/xemr

EPR Specialist Vignettes

Edited by
Arthur Schweiger

Magic Angle Spinning in Pulse EPR

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Introduction

Magic angle sample spinning (MAS) has revolutionized solid-state NMR spectroscopy. A search in the database of the Institute for Scientific Information reveals that in 1998 out of 1,312 papers on solid-state NMR, 689 (53%) explicitly mention MAS in their title, abstract, or keywords. This success story was not anticipated on introduction of the method in 1958 by Andrew et al.[1] and Lowe.[2] In fact, the experiment got a slow start. It was the first method to narrow dipolar broadened lines and was perceived as being very elegant from the very beginning. Yet it was also technically demanding, worked only for part of the samples that were of interest at that time, and was soon superseded for these samples by other methods of line narrowing like multi-pulse sequences. When in the 1970s the introduction of a new cross polarization technique by Pines, Gibby, and Waugh[3] gave access to solid-state ^{13}C NMR spectra, the sleeping beauty finally woke up. The present popularity of MAS in solid-state NMR is due to an often astonishing gain in resolution for powder samples and disordered systems. This is achieved by averaging the anisotropic terms in the Hamiltonian that are the most important contributions to the linewidth. Line broadening in EPR on such samples is also due to anisotropic terms in the Hamiltonian. It is therefore worth asking if high-resolution solid-state EPR can be based on the same idea.

This has long been considered to be impossible. To see why, we have to understand how MAS NMR works. It is basically an FT NMR experiment that starts with excitation of nuclear coherence (transverse magnetization) by a $\pi/2$ pulse. This coherence defocuses due to the anisotropic broadening, which is nothing else than a distribution of resonance frequencies.[4] After a full period of sample rotation, however, refocusing occurs. This is called a rotational echo. As anticipated by the pioneers,[1,2] such an echo is even formed for strongly dipolar coupled spectra, provided the spinning frequencies are sufficiently high.[5] Closer inspection shows that the refocusing of the anisotropic broadening in the rotational echo is *complete* if and only if the rotation axis includes the magic angle (54.74°) with the axis of the static field $\mathbf{B}_0$. This is because the anisotropic interactions can be described by second rank tensors whose orientation dependence is described by the Legendre polynomial $P_2=(3\cos^2\theta-1)/2$, which features a zero-crossing at the magic angle. The FID during MAS therefore consists of a series of rotational echoes whose amplitudes are modulated only by the isotropic parts of the interactions and decay with the phase memory time T_m. A Fourier transformation of this echo train yields an isotropic spectrum. In addition, so-called rotational sidebands are observed if the anisotropy of an interaction is larger than the sample spinning frequency. To obtain the isotropic spectrum with decent resolution, *several* rotational echoes have to be observed. This is why the experiment fails in the EPR case: Mechanical sample rotation cannot compete with our usual phase memory times T_m of at best a few microseconds.

Ultraslow in NMR, ultrafast in EPR

A few years ago, Hubrich and Spiess realized that a different incarnation of MAS, the so-called ultraslow MAS NMR or magic-angle turning experiment introduced in 1992 by Gan[6] might be feasible in EPR. This experiment makes clever use of the idea which goes back to Bax et al.[7] that it suffices to average the resonance frequencies of the spins at only three distinct orientations. This is easy to see for the special case where one principal axis of the interaction tensor is parallel to $\mathbf{B}_0$ at the start of the experiment. As the magic angle is also the angle between the axes of a cube and its diagonal, rotation by 120° aligns the next principal axis of the tensor with $\mathbf{B}_0$. Further rotation by another 120° does this for the third principal axis, so that the average of the three resonance frequencies corresponds to the average of the three principal values, which is nothing else than the isotropic part of the tensor. Indeed one can show that this works for *any* initial orientation of the tensor. The experiment can now be completed in two thirds of a sample rotation, and, in addition the magnetization can be stored during sample reorientation along z. Now a 240° reorientation of the sample has to

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compete only with longitudinal relaxation, and this is possible with advanced sample spinners.

In NMR this experiment is sometimes called ultraslow MAS, because the sample should ideally not move at all during the measurements of the three distinct frequencies. If the sample moves slowly enough, reorientation effects can be neglected for these measurements, and this means rotation frequencies below 200 Hz in NMR, whereas conventional MAS uses rotation frequencies in the kHz range. In EPR, all frequencies are by two to three orders of magnitude larger, so that spinning at the highest spinning frequencies applied in NMR results in ultraslow MAS in EPR. Since an EPR offset frequency can often be measured with sufficient precision in about a microsecond, reorientation during the measurement can be neglected in a fair approximation, even for MAS frequencies between 15 to 30 kHz. At the same time, such MAS frequencies are the upper limit of current MAS NMR technology and they are also sufficient to compete with T_1 for organic radicals at ambient temperature or slightly below that.

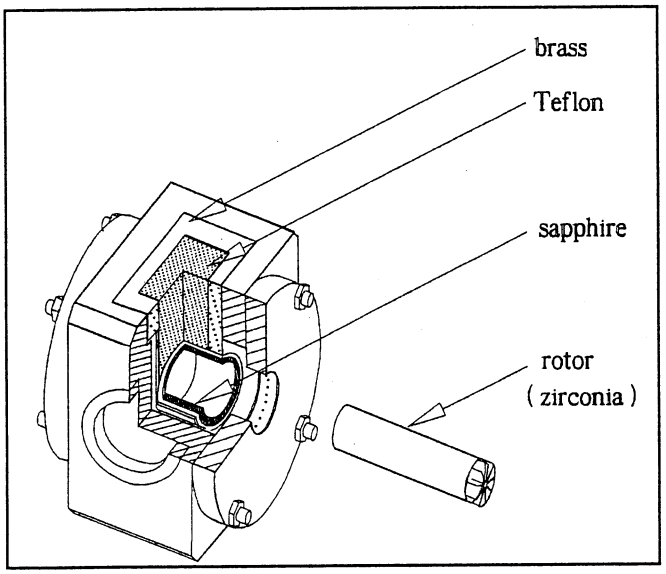

Fig. 1: Dielectric EPR resonator incorporated into a commercial MAS stator (Bruker). The outer diameter of the MAS rotor containing the sample is 4 mm. Rotor bearing and drive are by a nitrogen gas stream.

It remained to prove that an EPR probehead built around such a spinning device can be realized with sufficiently low microwave losses. Fig. 1 shows the technical solution by Hubrich, Bauer, and Spiess that succeeded. A sapphire dielectric ring is incorporated in a commercial MAS stator from Bruker, where normally the NMR coil would be positioned. The resonator and rotation axis are horizontal. As the direction of $\mathbf{B}_0$ in a standard X band EPR spectrometer is also horizontal, the angle between the rotation axis and $\mathbf{B}_0$ can be varied by turning the probehead around its long axis. With this setup and the pulse sequence displayed in Fig. 2, the authors could demonstrate line narrowing by MAS in the EPR spectrum of E_1' centers in γ-irradiated fused silica.[8]

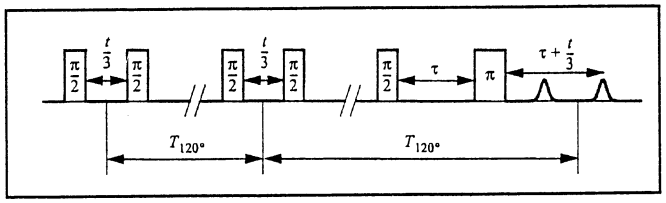

Fig. 2: Pulse sequence for the MAS EPR experiment. The amplitude of the second echo is observed while t is varied.

The pulse sequence is composed of three pulse pairs at the sample positions 0°, 120°, 240°. The first two pulse pairs excite electron coherence with a π/2 pulse, let it gain phase at the frequency corresponding to this position for time $t/3$, and store it along z. The third pulse pair is a variation with respect to the original NMR experiment that is necessary because we can observe only echoes, not FIDs in solid state EPR. Again, coherence is excited and then refocused by a π pulse. Because of the previous defocusing at the other positions, two echoes appear instead of only one, displaced by $t/3$ with respect to the usual echo position. The amplitude of the second echo is observed as a function of t, and this is modulated with the isotropic frequency. Fourier transformation of this echo modulation and computation of

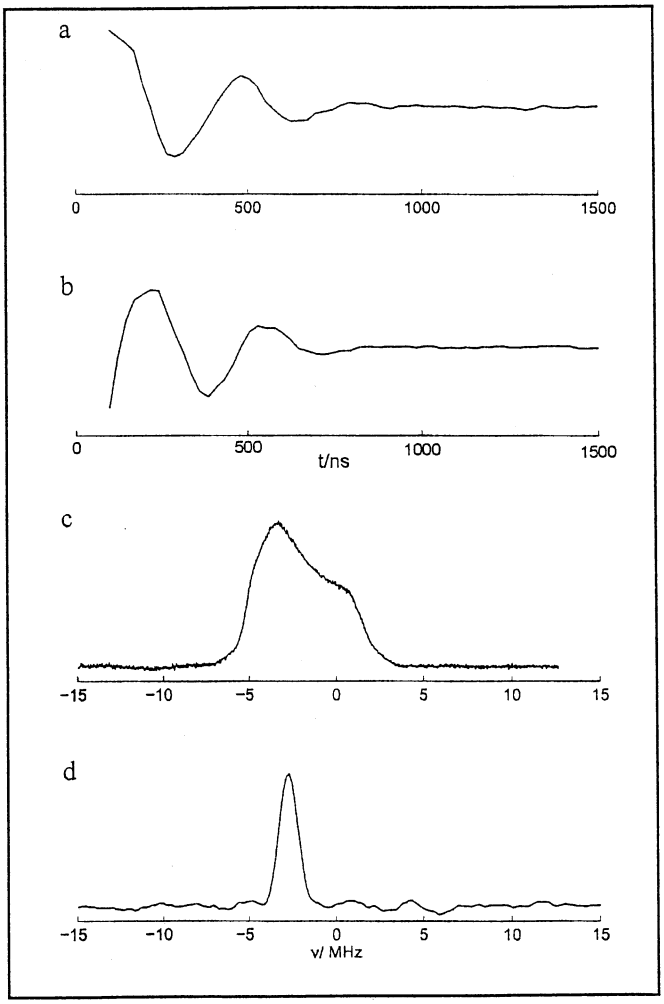

Fig. 3: MAS EPR on E_1' centers in γ-irradiated fused silica. a) Real part of the time domain data. b) Imaginary part of the time-domain data. c) Electron-spin echo detected EPR spectrum without MAS. d) Pure absorption MAS spectrum obtained by Fourier transformation of the data in a) and b) and phase correction.

the magnitude spectrum yielded the first MAS EPR spectrum. Meanwhile we have introduced a phase cycle that allows for quadrature detection and for proper phase correction, so that narrower absorption spectra are obtained. An example, again for E_1' centers in γ-irradiated fused silica is shown in Fig. 3.

Outlook

Now that MAS EPR is feasible, will it soon come to an EPR spectrometer near you? The answer is almost certainly no. This is because of a common problem in pulse EPR, the lack in excitation bandwidth. On first sight it might appear that this does not spoil the MAS EPR experiment except for some loss in sensitivity. The averaging of the anisotropic interactions works for each single spin packet, so that those spin packets that can be excited at all three rotor positions should still contribute to the isotropic spectrum. The signal from other spin packets would simply be lost. However, closer inspection reveals that the different spin packets lead to signal contributions with significantly different phases if the excitation bandwidth is small compared to the width of the spectrum. The signal then is further reduced due to destructive interference. Our experiments on the E_1' centers and on γ-irradiated sulfamic acid show that MAS EPR can be observed for $1/t(\pi/2)>\Delta\omega$, where $t(\pi/2)$ is the length of a $\pi/2$ pulse and $\Delta\omega$ the width of the whole spectrum. With current microwave technology, this condition can be fulfilled only for a few organic radicals and defect centers. Therefore, MAS EPR at present cannot compete with other methods for resolution enhancement like ENDOR, which are easier to implement.

This somewhat pessimistic view, however, does not cover the full scope. Fast sample spinning is also required if experiments in the spirit of anisotropy-resolved EPR by Sierra and Schweiger[9,10] are to be applied to organic radicals. Our first tests with such an approach are encouraging. Sensitivity is good, resolution enhancement significant, and excitation bandwidth limitations do not spoil these experiments. After all, fast sample spinning might still find its way into routine use in pulse EPR.

Acknowledgment

The author is grateful to M. Hubrich and H.W. Spiess for many discussions on the birth of MAS EPR and C. Bauer for discussions on the probeheads and for providing Fig. 1. Thanks are also due to D. Hessinger who explored the limits of MAS EPR and worked on further applications of fast sample spinning that will be published elsewhere.

References

1. E.R. Andrew, A. Bradbury, and R.G. Eades, Nature 182, 1659 (1958); ibid. 183, 1802 (1959).
2. I. Lowe, Phys. Rev. Lett. 2, 285 (1959).
3. A. Pines, M.G. Gibby, and J.S. Waugh, J. Chem. Phys. 56, 1776 (1972); ibid. 59, 569 (1973).
4. Things are a little bit more complicated for *homogeneous* anisotropic broadening due to homonuclear couplings, but here we have in mind only chemical shift anisotropy and heteronuclear couplings that are analogous to *g* anisotropy and hyperfine couplings in EPR.
5. C. Filip, S. Hafner, I. Schnell, D. E. Demco, and H.W. Spiess, J. Chem. Phys. 110, 423 (1999).
6. Z. Gan, J. Am. Chem. Soc. 114, 8307 (1992).
7. A. Bax, N.M. Szeverenyi, and G.E. Maciel, J. Magn. Reson. 52, 147 (1983).
8. M. Hubrich, C. Bauer, and H.W. Spiess, Chem. Phys. Lett. 273, 259 (1997).
9. G.A. Sierra and A. Schweiger, Rev. Sci. Instrum. 68, 1316 (1997).
10. G.A. Sierra and A. Schweiger, Mol. Phys. 95, 973 (1998).

TIPS & TECHNIQUES

Preparation and Use of a Magnetic Field Set and Sweep Standard

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The magnetic field of an EPR spectrometer can be determined with an accuracy of $1/10^5$ - $1/10^6$ by use of an NMR gaussmeter, the precision depending on the homogeneity of the field and the physical size of NMR probe and whether a correction for the chemical shift of the proton standard is applied. However, unless the NMR probe is at the same position as the sample within the microwave cavity, a significant error in field measurement can result, as much as 0.1 mT depending on the magnet and the relative placement of the probe external to the cavity. Bruker markets a small in-cavity probe for this purpose. More commonly, one places the NMR probe alongside the cavity during EPR measurement and corrects for the difference between the field at the probe and at the sample due to the field strength variation across the magnet gap and the influence of the cavity structure on the field. For our 9.5″ magnet with a 2.22″ gap and at a field strength of 326.8 mT, the field measured alongside a Varian TE_{102} rectangular cavity is 0.017 mT smaller than at the sample. However, for most purposes it is more convenient (especially with older generation spectrometers) and equally accurate to employ a

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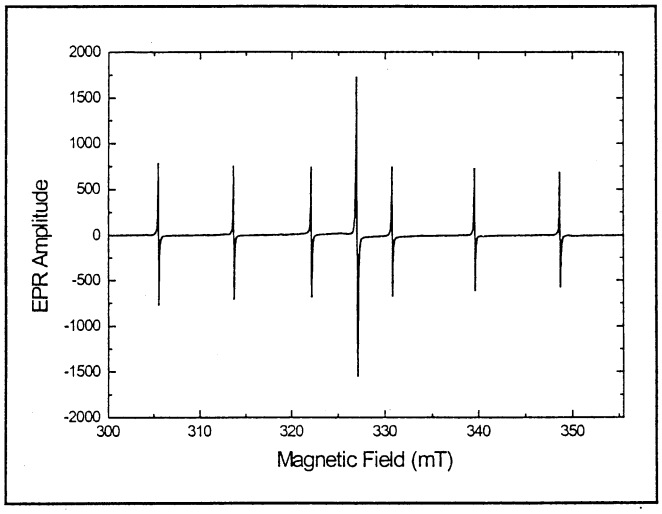
standard sample and microwave frequency counter to calibrate the field. At X-band (~9.5 GHz), the frequency stability of the cavity at room temperature is typically $\pm 10^{-4}$ GHz ($1/10^5$) or better and the accuracy in the g-factor for powdered radical standards is about ± 0.0001 ($5/10^5$) and for solution radical standards about ± 0.00002 ($1/10^5$). Thus, the absolute value of the magnetic field strength can be calibrated to ± 0.015 mT using an easily prepared and stable powder standard and a microwave frequency counter. This level of accuracy is sufficient for most work with radicals and transition metal ions having peak-to-peak linewidths $\Delta B_{pp} \geq$ 0.1 mT. A number of field strength (g-factor) and sweep (hyperfine splittings) calibration standards are described in books on EPR (1,2).

Here we describe the preparation and characterization of a Mn(II)/CaO/coal standard sample that we use routinely in our laboratory for calibrating the field set and field sweep on our X-band and Q-band spectrometers. The sample is easy to make and is stable when sealed in an EPR tube under vacuum. Most alkaline oxides exhibit 6-line Mn(II) EPR spectra from impurities in sites of O_h symmetry. Mn(II) in SrO has long been suggested as a field sweep standard (1). We have chosen CaO because it is more widely available and one can usually find a sample with a Mn(II) EPR signal of suitable intensity. We have used reagent grade CaO, although blackboard chalk ($CaCO_3$) when heated at 500 °C for several hours produces CaO with a suitable EPR spectrum. Normally, we anneal reagent grade CaO at 500 °C for 3 hr to sharpen the EPR lines and to remove any $CaCO_3$ formed from reaction of the CaO with atmospheric CO_2 over time. The manganese lines of samples prepared in this way have line widths, ΔB_{pp}, that vary from 0.060 to 0.070 mT across the sextet from low to high field.

The CaO sample is blended with a trace amount of coal with a mortar and pestle. We have used Burbh blacksvill #2 which gives a single line at g = 2.0035 in the middle of the Mn(II) sextet (see Figure). The CaO/coal blend is packed in a 3 mm i.d.- 4 mm o.d. quartz EPR tube and sealed under vacuum and the g-factor of the coal determined. The line width of Burbh blacksvill #2 coal is narrowed from about $\Delta B_{pp} = 0.4$ mT in air to 0.17 mT under vacuum. Other coal samples used in EPR oximetry, for example selected gloxy having a linewidth of only 0.085 mT under vacuum (3), could also be used but one should always determine the g-factor after evacuating the sample, not before. A number of coals are available from the Argonne Premium Coal Samples



Program (http://www.anl.gov/PCS/pcshome.html). If coal is not included in the standard, the Mn^{2+}/CaO is simply flame sealed at atmospheric pressure to keep out moisture and CO_2. A vacuum is required for samples containing coal because the signal does not have long-term stability due to slow oxidation of the coal radicals, causing changes in line shape and g-factor as well as intensity of the EPR signal.

We prefer to use the single line of coal as a field set standard since the large hyperfine splitting of the Mn^{2+} sample requires third-order corrections to line positions (4) and nonlinear field sweeps can introduce errors in measured values of B_o. Table I summarizes the spin Hamiltonian parameters for Mn^{2+} in CaO and for our coal at room

TABLE I: SPIN-HAMILTONIAN PARAMETERS

Temperature	g_o ($^{55}Mn^{2+}$)	a_o ($^{55}Mn^{2+}$), mT	A_o ($^{55}Mn^{2+}$), 10^{-4} cm^{-1}	g_o (coal)
RT	2.0011(1)	8.627(4)	80.62(3)	2.0035(1)

TABLE II: SPAN BETWEEN PAIRS OF Mn^{2+} HYPERFINE LINES

Temperature	Span ($M_I = \pm 1/2$) Lines	Span ($M_I = \pm 3/2$) Lines	Span ($M_I = \pm 5/2$) Lines
Room Temp.	8.627(4), mT	25.881(4), mT	43.133(4), mT
77 K	8.721(4)	26.167(4)	43.573(4)

temperature. The parameters agree with the literature values at 295 K for Mn^{2+} in CaO (5) although the values reported here are to greater precision.

In our laboratory, the Mn^{2+} spectrum is used primarily for calibrating the field sweep at X-band. At Q-band (35 GHz), the spectrum is first-order and thus is a useful g-mark at the higher frequency. The field spans between symmetrical pairs of Mn^{2+} lines having the same $|M_I|$ are given in Table II at room temperature and at 77 K. Over the past 20 years, we have measured the Mn^{2+} spectra of various CaO samples using a number of different EPR spectrometers, microwave frequency counters and NMR gaussmeters and have consistently obtained the results in Table II within the stated errors.

We also use the Mn^{2+}/CaO/coal sample as a standard for measurement of g-factors and hyperfine splittings when using a TE_{104} dual cavity (6). In this application, two standard samples are needed to determine the difference in field experienced by the two halves of the dual cavity or to adjust the position of the cavity within the magnet gap so that the field is identical at the sample positions in both halves.

Acknowledgment:

We thank Dr. Ira Goldberg of Rockwell International for independently measuring the Mn^{2+}/CaO spectrum in his laboratory and verifying the results obtained here. This work was supported by NIH grant R37 GM 20194.

References:

1. H.M. Swartz, J.R. Bolton and D.C. Borg, "Biological Applications of Electron Spin Resonance" Wiley Interscience, 1972, New York, pp 98-101.
2. J.A. Weil, J.R. Bolton and J.E. Wertz, "Electron Paramagnetic Resonance. Elementary Theory and Practical Applications", John Wiley & Sons, Inc., 1994, New York, pp 510-513.
3. K.J. Liu, M. Miyake, P.E. James and H.M. Swartz (1998), *J. Magn. Reson.* **133**, 291-298.
4. G.D. Markham, B.D. Nageswara Rao, and G.H. Reed (1979), *J. Magn. Reson.* **33**, 595-602.
5. J. Rubio O., E. Muñoz, J. Boldú O., Y. Chen and M.M. Abraham (1979), *J. Chem. Phys.* **70**, 633-638.
6. Q.-Y. He, A.B. Mason, R.C. Woodworth, B.M. Tam, R.T.A. MacGillivray, J.K. Grady and N.D. Chasteen (1997), *Biochemistry* **48**, 14853-14860.

REPORTS & PROCEEDINGS

Report on the Eighth Annual Workshop: "Modern Development of Magnetic Resonance" 22-24 September 1999, Kazan, Tatarstan

The program of the Workshop was as follows: L.S. Sochava (Ioffe Physical Technical Institute, St.-Petersburg, Russia) *An alignment of axial paramagnetic centers in crystals induced by anisotropic photo ionization.* M.S. Tagirov (Kazan State University, Kazan, Russia) *Magnetic resonance in van Vleck paramagnets.* Yu.V. Yablokov (Zavoisky Physical-Technical Institute, Kazan, Russia) *About role of excited vibronic states in Jahn-Teller dynamics.* M. Krupski (Institute of Molecular Physics, Poznan, Poland) *EPR under high pressure - technique and applications.* M.M. Zaripov, V.A. Ulanov, (Zavoisky Physical-Technical Institute, Kazan, Russia) *Linear impurity microstructures in SrF_2 and BaF_2 crystals: Study by EPR.* M. Belinskii (Tel-Aviv University, Tel-Aviv, Israel) *Exchange effects in EPR and hyperfine parameters of polynuclear metal centers in biological systems and model compounds.* M.L. Falin, K.I. Gerasimov (Zavoisky Physical Technical Institute, Kazan, Russia) B.N. Kazakov (Kazan State University, Kazan, Russia) *Spectrometer for optical detection of magnetic resonance: Magneto-optical study of Yb^{3+} in BaF_2 single crystal.* E. Reijerse (University of Nijmegen, Nijmegen, The Netherlands) *High-frequency EPR of high-spin systems - theory and applications.* N.N. Garif'yanov (Zavoisky Physical-Technical Institute, Kazan, Russia) *Investigation of the electronic properties of sodium-tungsten bronzes.* M.L. Falin, V.A. Latipov (Zavoisky Physical-Technical Institute, Kazan, Russia), B.N. Kazakov, A.M. Leushin (Kazan State University, Kazan, Russia), H. Bill, D. Lovy (University of Geneva, Geneva, Switzerland) *EPR, ENDOR and optical spectroscopy of the*

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tetragonal Yb^{3+} centers in $KMgF_3$. J.H. van der Waals (Leiden University, Leiden, The Netherlands) *EPR study of an old problem: The nature of the luminescent state of the d0 transition metal tetroxo anions.* S. Yamauchi (Institute for Chemical Reaction Science, Tohoku University, Sendai, Japan). *Multidimensional and multifrequency EPR on excited multiplet states.* A. Krushelnitsky, V. Fedotov, (Kazan Institute of Biochemistry and Biophysics, Kazan, Russia), D. Reichert, H. Schneider (Halle University, Halle, Germany), *Solid state MAS exchange NMR spectroscopy and superslow protein dynamics.*

In the morning of September 24, a reception of Professor J.H. van der Waals by the Prime-Minister of the Republic of Tatarstan R. Minnekhanov took place.

The Zavoisky Award was presented September 24, 1999 in Kazan, the capital city of the Republic of Tatarstan. It was there that academician E.K. Zavoisky discovered EPR in 1944. The Zavoisky Award consists of a Diploma, a Medal and one thousand US dollars. The Zavoisky Award was established by the Zavoisky Physical-Technical Institute of the Russian Academy of Sciences with support from the Kazan State University, the Springer-Verlag Publishing House, the Republic of Tatarstan, the Tatarstan Academy of Sciences, the AMPÉRE Society and the International EPR Society. The Award Selection Committee consisted of well-known experts in EPR: Professors B. Bleaney (Oxford), G. Feher (La Jolla), K. Möbius (Berlin), A. Schweiger (Zurich), Yu.D. Tsvetkov (Novosibirsk), and the Chairman K.M. Salikhov (Kazan). The selection of the Awardee was made after consultations with the Advisory Award Committee which comprises: K.H. Hausser (Heidelberg), C.A. Hutchison Jr. (Chicago), and Yu.N. Molin (Novosibirsk).

Previous winners of the Zavoisky Award were: W.B. Mims (1991), B. Bleaney (1992), A. Schweiger (1993), J.R. Norris, Ya.S. Lebedev and K. Möbius (1994), J.S. Hyde (1995), G. Feher (1996), K.A. Valiev (1997), and J.H. Freed (1998). The Organizing Committee owes special thanks to the NIOKR Fund of the Republic of Tatarstan, and the Russian Fund for Basic Research.

Conference Report

Second Asia-Pacific EPR/ESR Symposium

The 2nd Asia-Pacific EPR/ESR Symposium (APES'99) was held, under the auspices of the Asia-Pacific EPR/ESR Society (APES), at the Zhejiang University, Hangzhou, China, from October 31 through November 4, 1999. The Symposium was attended by about 117 participants from 17 different countries, among whom 75 were from Asia-Pacific, Europe and North America, whereas 42 were from China (including Hong Kong). At the Opening Ceremony, Prof. Yuri Tsvetkov has been presented the 1999 IES Silver Medal in Chemistry by Prof. John R. Pilbrow, President of the International EPR/ESR Society (see separate note).

The meeting featured the following plenary lectures: Prof. H.M. Swartz, *In Vivo EPR: Opportunities and Challenges*; Prof. J.R. Pilbrow, *EPR of Disorder Systems*; Prof. Z. Liu, *Kinetic EPR Studies on Bio-antioxidants*; Prof. G.R. Eaton, *Perspectives on Spins – The Relaxation Domain*; Prof. M. Motokawa, *Electron Spin Resonance of Magnetic Materials in High Fields and High Frequencies*; Prof. K.M. Salikhov, *The potential for using observer spins to investigate charge separated states in photo-synthesis*; Prof. M. Che, *Insight into the Chemistry of Oxide Surfaces by means of EPR Techniques*; Prof. H. So, *Metal-Oxygen Clusters Containing*

One, Two, or Three Unpaired Electrons; Prof. L. Kevan, *Pulsed Electron Magnetic Resonance of Transition Metal Ions in Microporous and Mesoporous Oxide Materials*. The following invited talks were also given: Prof. S. V. Bhat, *ESR Evidence for Symmetry Conservation During Radiation Damage - III Rotational Symmetry Conservation in X-Irradiated Single Crystals of* $LiClO_4 \times 3H_2O$; Prof. Y. Tsvetkov, *Pulsed Electron Double Resonance and Its Applications*; Prof. K. Kuwata, *Studies on Photochemical Reactions by FT-ESR*; Prof. J.-J. Yin, *Ti Sensitive Spin Label ESR Technique and Its Applications in Membrane Biophysics Study*; Prof. A. Rockenbauer, *Decomposition of Multi-Component EPR Spectra*; Prof. K.P. Mishra, *Fluorescence and ESR Studies on Membrane Oxidative Damage by Gamma Radiation*; Prof. Y. Liu, *ESR Investigation on Semiquinone Radicals in The Reactions Between Phenolic Antioxidants Isolated From Natural Plants and Superoxide Anion Radicals*; Prof. K.-J. Liu, *Challenges and Opportunities of Trapping and Detecting Free Radicals In Vivo*.

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 containing the selected papers will be published in a forthcoming issue of *Applied Magnetic Resonance* with Prof. Y. Xu as the Guest Editor.

During the Symposium the 2nd Meeting of the Asia-Pacific EPR/ESR Society was held. We were privileged to have with us Prof. John R. Pilbrow, President of the International EPR/ESR Society, who delivered an Address to the participants of the Meeting. The 37 researchers from Asia-Pacific region present have elected the APES Council as follows: President: Prof. C. Rudowicz; Vice-President: Prof. A. Kawamori (Japan); Secretary: Dr Y.Y. Yeung (Hong Kong); Treasurer: (it was decided that in view of adopting free membership, the position of Treasurer was not required for this term); Representatives from: Australia/New Zealand: Dr. G. Hanson; Japan: Prof. H. Ohta; P. R. China: Prof. Y. Li; India: Prof. S.V. Bhat; Rep. of Korea: Prof. H.S. So; Vietnam: Prof. T.T. Nguyen; Russia - Far East: Prof. A. Ziadtinov. Endorsement for the elected Council will be sought from the APES members who could not attend APES'99. An e-mail and postal ballot will be conducted before January 2000.

It was decided at the APES Meeting that the third Symposium (APES'01) will be held in Kobe in October/November 2001, with Prof. A. Kawamori as the Chairman and Prof. H. Ohta as the Secretary of the Local Organising Committee (LOC) for APES'01, respectively, whereas the fourth Symposium (APES'03) will be held in Bangalore in October/ November 2003 with Prof. S.V. Bhat as the Chairman of the LOC. An EPR/ESR Workshop or a School with tutorial sessions for students and researchers is also planned to be held before the APES'03. All materials related to the APES'99 as well as the APES Meeting are available on the APES Web site at:

http://www.ied.edu.hk/has/phys/apepr

For updated information on the future Asia-Pacific EPR/ESR Symposia please visit the APES Web site.

On behalf of the APES Council I would like to thank all hard working Members of the APES'99 Local Organising Committee for their dedicated effort as well as the sponsoring organisations who financially supported the Symposium. Under the skilful leadership of Prof. Yuanzhi Xu, the APES'99 have been a very successful Symposium. In the appreciation of the commitment and hard work, Professor Xu and each member of his team has been awarded the APES Distinguished Service Award, which were presented by the President of the Asia-Pacific EPR/ESR Society at the Closing Ceremony during the Symposium Banquet.

Czeslaw Rudowicz
President , The Asia-Pacific EPR/ESR Society

UPDATE

Present and Future of HF EPR Instrumentation
Proceedings published in *Applied Magnetic Resonance*

Manuscripts from the March 1998 conference "International Experts' Workshop on the Present and Future of HF EPR Instrumentation" were published in Volume 16 #2 of *Applied Magnetic Resonance*. We have learned this issue may be ordered separately for DM230 (approximately $122 USD) plus postage. To order, contact Springer-Verlag

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

Wien New York, Subscription Department, Sachsenplatz 4-6, A-1200 Wien, Austria (FAX: 43-1-330-24-26-62; E-mail: journals@springer.at. There is free access to the table of contents and the abstracts of the issues on the journal's homepage:

http://www.springer.at/amr

For those who wish to subscribe for a full year, the discounted cost for IES members in good standing is $155 USD plus $54 USD postage for a year 2000 subscription .

Mechanisms of High Temperature Superconductivity (HTSC)
by Peter Brusov

Rostov State University Publishing has published the monograph *Mechanisms of High Temperature Superconductivity (HTSC)* by Peter BRUSOV (two volumes, hard cover, 1383 pages, in English, price US$184 + US$15 postage for both volumes). This is the first attempt to represent most of the mechanisms of HTSC, making this book like an encyclopedia of HTSC theory. The monograph will be useful for both theoretists and experimentalists studying different aspects of HTSC as well as for graduate and postgraduate students interested in HTSC. For information on ordering this book, send an e-mail message to Peter Brusov at pnb@rnd.runnet.ru.

NOTICES of MEETINGS

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

INTERNATIONAL SOCIETY for MAGNETIC RESONANCE in MEDICINE 8th SCIENTIFIC MEETING and EXHIBITION, Denver, Colorado, April 1-7, 2000.

The Eighth Scientific Meeting of the International Society for Magnetic Resonance in Medicine will take place 1-7 April 2000 at the Colorado Convention Center in Denver, Colorado, USA.For full details, please contact the ISMRM office, ☎: 1-510-841-1899, e-mail: info@ismrm.org; or visit the Society's web page:

http://www.ismrm.org/

HIGH-FREQUENCY ELECTRON PARAMAGNETIC RESONANCE: TECHNOLOGY and APPLICATIONS, Amsterdam, The Netherlands, April 12-14, 2000.

This conference is being organized under the auspices of the Academy Committee for Chemistry of the Royal Netherlands Academy of Arts and Sciences. The local organizing committee consists of Peter Gast, Edgar Groenen, Arnold Hoff, and Jan Schmidt. The aim of the conference is to report on the progress in the technology of High-Frequency EPR and on applications in physics, chemistry and biology. The program will consist of invited and contributed lectures and poster presentations. A brochure accompanies this newsletter. Scientists interested in contributing to or participating in this conference are invited to contact the web page:

http://www.knaw.nl/hfepr

For further information contact Mr. R. des Bouvrie, Royal Netherlands Academy of Arts and Sciences, P.O. Box 19121, 1000 GC Amsterdam, The Netherlands; E-mail: roy.des.bouvrie@bureau.knaw.nl; ☎: 31-20-55-10-730; FAX: 31-20-62-04-941.

3rd WORKSHOP ON EPR INSTRUMENTATION AND METHODOLOGY, National Biomedical EPR Center Biophysics Research Institute, Medical College of Wisconsin, Milwaukee, Wisconsin, May 5-6, 2000.

Our Third Workshop on EPR instrumentation and methodology will be held Friday and Saturday, May 5 and 6, 2000. The title of this workshop is "EPR Methods in Structural Biology." The first day will consist of lectures, while the second day will be devoted to hands-on demonstrations, discussions, and tours of the National Biomedical EPR Center.

This workshop is supported by the National Center for Research Resources of the National Institutes of Health. The workshop will mark the 25th year of funding for the National Biomedical EPR Center by NCRR.

The budget for the workshop is limited, but it is expected that a portion of the living expenses while attending the

Conference will be covered. Also, a limited number of travel awards for students may be available.

If you are interested in attending, please contact Christopher C. Felix, Ph.D., Scientific Administrator, 8701 Watertown Plank Road, P.O. Box 26509, Milwaukee, WI 53226-0509, USA; ☎: 414-456-4000, Fax: 414-456-6512, E-mail: cfelix@mcw.edu

42nd ROCKY MOUNTAIN CONFERENCE ON ANALYTICAL CHEMISTRY; 23rd INTERNATIONAL EPR SYMPOSIUM, Broomfield, Colorado, July 30-August 3, 2000.

Sponsored by the Rocky Mountain Section Society for Applied Spectroscopy and the American Chemical Society Colorado Section. Major Symposia on EPR and NMR are held at this conference. Details will be published in future editions of this newsletter, or visit the following web site:

http://www.milestoneshows.com/events.html

XIXth INTERNATIONAL CONFERENCE on MAGNETIC RESONANCE in BIOLOGICAL SYSTEMS (XIX ICMRBS), Florence, Italy, August 20-25, 2000.

You are cordially invited to attend the XIXth International Conference on Magnetic Resonance in Biological Systems (XIX ICMRBS) to be held in Florence, Italy from August 20 to 25, 2000. Florence is easily accessible both by train (ca. 1.5 hrs from Rome by fast train) and by plane. The airport, located 5 Km from the city center, is connected, through direct flights, with the major Italian and European cities.

Scientific Program–The scientific program will cover a wide range of research topics in the field of magnetic resonance applied to biological systems. Particular attention will be devoted to new and promising areas of research as well as to emergent methodological tools within the frame of NMR research in the post-genomic era. The scientific agenda will include plenary lectures, session lectures and poster presentations. The sessions will be organized on the following topics: protein structure, folding, and mobility; EPR/ENDOR applications; membrane proteins; In vivo spectroscopy and imaging; DNA, RNA, nucleotides and their interaction with proteins; SAR of drugs and drug discovery; computation and dynamics.

Location–The conference will take place at the Centro Internazionale Congressi and Palaffari Firenze located close to the central railway station in the historical and monumental area of Florence.

Accommodation–Accommodation will be arranged in hotels of different categories, mostly within walking distances from the venue (student dorms will be available). Detailed information and reservation forms for accommodation will be included in the second circular.

Change of Address–Information on the scientific program, accommodation, general arrangements, registration forms and instructions for preparation of abstracts are continuously updated in our web site. Please visit it! Registration can be done on line. Abstract and early registration deadline is March 31, 2000. For further information, please contact the XIX ICMRBS Secretariat, Dept. Chemistry & CERM, Univ. Florence, Via Luigi Sacconi 6, I-50019 Florence, Italy; ☎: 39-055-4209260; Fax: 39-055-4209253; E-mail: icmrbs@cerm.unifi.it. Or visit the web address at:

http://www.cerm.unifi.cnr.it//icmrbs.html

Conference Committees: *Organizers:* I. Bertini, (Florence, Italy) Chairperson; L. Banci (Florence, Italy) Ex. Manager; R. Kaptein (Utrecht, The Netherlands); H. Rueterjans (Frankfurt, Germany); G. Valensin (Siena, Italy). *Assistants to the organizers*: R. Del Conte & I.C. Felli (Florence, Italy); Treasurer: P. Turano (Florence, Italy). International Advisory Board: A.S. Arseniev (Moscow, Russia); C.M. Dobson (Oxford, U.K.); S. Forsen (Lund, Sweden); G. Govil (Bombay, India); A.M. Gronenborn (Bethesda, USA); C.W. Hilbers (Nijmegen, The Netherlands); J.S. Hyde (Milwaukee, USA); C. Ho (Pittsburgh, USA); M. Kainosho (Tokyo, Japan); J.F. Lefevre (Strasbourg, France); J.L. Markley (Madison, USA); A. McDermott (New York, USA); K. Möbius (Berlin, Germany); R.S. Norton (Parkville, Australia); S.J. Opella (Philadelphia, USA); M. Rico (Madrid, Spain); J. Seelig(Basel, Switzerland); B.D. Sykes (Edmonton, Canada); W. Tang (Nanjing, China); G. Varani (Cambridge, U.K.); A. Walker (Tucson, USA). *National Organizing Committee*: Coordinator: A. Rosato (Florence, Italy); S. Aime (Torino); R. Basosi (Siena); R. Bazzo (IRBM); F. Conti (Roma); A. Di Nola (Roma); A. Lai (Cagliari); S. Mammi (Padova); B. Maravigila (Roma); C. Marchioro (Glaxo); G. Martini (Firenze); H. Molinari (Verona); V. Pavone (Napoli); A. Perico (CNR, Italy); F. Podo (Ist. Sup. Sanita); A. Rigo (Padova); A.L. Segre (CNR); A. Spisni (Parma); M. Tato' (Pharm.& Upjohn); P.A. Temussi (Napoli); A. Tomasi (Modena); A. Tramontano (IRBM); F. Uggeri (Bracco); L. Zetta (CNR). *Chairperson of Local Organizing Committee:* R. Pierattelli (Florence, Italy).

6TH INTERNATIONAL SYMPOSIUM on SPIN TRAPPING: "SPIN TRAPS, NITROXIDES and NITRIC OXIDE SPECTROSCOPY, CHEMISTRY and FREE RADICAL BIOLOGY, Marseille, France, August 27-31, 2000.

Tentative Topics–The Scientific Committee has selected a broad range of topics: •Synthesis of novel nitroxides; •Synthesis of novel nitrones and nitroso spin traps; •Synthesis of nitric oxide and peroxynitrite donors; •Nitric oxide and peroxynitrite traps; •Spin trapping of superoxide and nitric oxide derived from nitric oxide synthases; •*In vivo* trapping of nitric oxide; •Pharmacokinetics of spin traps and spin adducts, bioreduction of nitroxides; •Nitroso hemoglobin; •Nitrone traps: antagonists of neuronal injury, ALS, and neurodegenerative diseases; •Chemistry and biology of nitroxyl anion.

Location–It is a great honour that Marseille has been chosen as the conference site. Marseille has a reputation for hospitality towards people from all nations. Its geographic location and ready accessibility offers a convenient and pleasant setting to host an international meeting.

We hope to match the excellence of the scientific sessions with an enjoyable and memorable social programme. We look forward to seeing you in Marseille in the year 2000.

Scientific Committee: A. Alberti *(Univ. Bologna, Italy)*; O. Augusto *(Univ. São Paulo, Brazil)*; M. Davies *(Heart Research Inst. at Sydney, Australia)*; B.C. Gilbert *(Univ. York,*

UK); L. Greci *(Univ. Ancona, Italy)*; K.U. Ingold *(Natl. Research Council at Ottawa, Canada)*; B. Kalyanaraman *(Medical Coll. Wisconsin, USA)*; K. Makino *(Univ. Kyoto, Japan)*; R.P. Mason *(NIEHS, USA)*; A. Rassat *(Ecole Normale Supérieure, Paris, France)*; A. Tomasi *(Univ. Modena, Italy)*; P. Tordo *(Univ. Provence, Marseille, France)*; J.L. Zweier *(Johns Hopkins Medical Inst., Baltimore, USA)*.

Local Organization: Prof. Paul Tordo and the memberships of *VMR 6517 "Chimie, Biologie et Radicaux Libres"* (association CNRS and Aix-Marseille 1 & 3 Universities).

Congress Secretariat: Atout Organisation Science, 6th International Symposium on Spin Trapping, 106 Corniche Kennedy, 13007 Marseille, France; ☎: 33-0-4-91-52-75-10; FAX: 33-0-4-91-52-93-73; E-mail: atoutsci@atout-org.com; or, for full meeting information visit the Congress web-site:

www.up.univ-mrs.fr/~wsrep/spin.trapping.meeting.html

AMPÉRE SUMMER SCHOOL on "APPLICATIONS of MAGNETIC RESONANCE in NOVEL MATERIALS," Nafplion, Peloponese-Greece, September 3-9, 2000.

The Ampére Summer School on "Applications of Magnetic Resonance in Novel Materials" will be held at Nafplion (Peloponese-Greece) 3-9 September 2000. The scope of the School is to introduce magnetic resonance techniques and their use in the investigation of current topics of Materials Science: 1) Disordered Systems and Glassy Materials; 2) Liquid Crystals; 3) Modulated and Incommensurate Systems; 4) Novel Electronic Conductors; 5) Ferromagnetic and Paramagnetic Systems; 6) Porous Systems; 7) Imaging of Materials; and 8) Bio-materials. Apart from NMR and MRI techniques, EPR and Mössbauer Spectroscopy will be also introduced.

The scientific program includes invited plenary lectures, oral and poster contributions. Young scientists are strongly encouraged to participate in the school and present their research activities in oral and poster contributions. The following lecturers will present one-hour plenary lectures: •Prof. Jersy S. Blicharsky *(Krakow, Poland)*; •Prof. Robert Blinc *(Ljubljana, Slovenia)*; •Prof. Bernhard Blumich *(Aachen, Germany)*; •Prof. Ferdinando Borsa *(Ames, Iowa)*; •Prof. Detlef Brinkman *(Zürich, Switzerland)*; •Prof. H. J. M. De Groot *(Leiden, Netherlands)*; •Dr. Jannis Deligiannakis *(Athens, Greece)*; •Prof. Jani Dolinsek *(Ljubljana, Slovenia)*; •Prof. Franz Fujara *(Dortmund, Germany)*; •Dr. Jorge Luis Gavilano *(Zürich, Switzerland)*; •Prof. Clare Gray *(NY, USA)* -not yet confirmed; •Prof. Mladen Horvatic *(Grenoble, France)*; •Prof. Kazushi Kanoda *(Tokyo)*-not yet confirmed; •Prof. Raymond Kind *(Zürich, Switzerland)*; •Prof. Serge Lacelle *(Quebec, Canada)*; •Prof. Fanny Milia *(Athens, Greece)*; •Prof. Pierre Panissod *(Strasbourg, France)*-not yet confirmed; •Prof. Moshe Paz-Pasternak *(Tel Aviv, Israel)*; •Prof. Vasilis Papaefthymiou *(Ioannina, Greece)*; •Dr. Josef Roos *(Zürich, Switzerland)*; •Dr. Josef D. Seymour *(Albuquerque, USA)*; •Prof. Jan Stankowski *(Poznan, Poland)*; •Prof. Josef Zwanziger *(Indiana, USA)*.

The School will be held at XENIAS PALLAS hotel, which rises above the town of Nafplion, at the southern coast, and is built in the middle-age castle of Akronafplia. Social and cultural events, as well as an official dinner will be arranged for the participants and the accompanying persons. For on-line registration and more information about the summer school and the town of Nafplion, please visit the web site of the Summer School at:

www.ims.demokritos.gr/nmrlab/conference/

For more information, please E-mail G. Papavassiliou at gpapav@ims.demokritos.gr

33rd ANNUAL INTERNATIONAL MEETING ESR GROUP of the ROYAL SOCIETY of CHEMISTRY and 4th MEETING of EUROPEAN FEDERATION of EPR GROUPS (EFEPR). A COMBINED MEETING on PROSPECTS for EPR SPECTROSCOPY in the 21st CENTURY, September 10-14, 2000, John Innes Centre, University of East Anglia, Norwich, UK.

More complete details will be published in the next issue of the *EPR Newsletter*, but full meeting details may be viewed on the following web page:

http://www.cf.ac.uk/esr/norwich.html

All application forms, abstracts or requests for further information should be sent to Dr. D.M. Murphy, Department of Chemistry, Cardiff University, PO Box 912, Cardiff CF10 3TB, UK. E-mail: MurphyDM@cardiff.ac.uk; ☎: 44 (0)1222 875850 or 874080; Fax: 44 (0) 1222 874030.

POSITIONS AVAILABLE & WANTED

POST-DOCTORAL POSITION AVAILABLE at the TOKYO INSTITUTE of TECHNOLOGY

The Tokyo Institute of Technology is seeking applications from appropriate candidates for a JSPS (Japan Society of Promotion of Sciences) Post Doc. The requirements for this position are: a Ph.D. earned after April 1993 and US citizenship (or green card). He or she is requested to come to Japan by the end of March, 2000. The contract will be one + one year, for two years max. (minimum 3 months, maximum 2 years). Monthly salary is 270 (+ 50 for accompanying family) kyen, about US$2,550 (+ US$480). In addition, 200 kyen will be paid at the time of arrival and up to 100 kyen (US$940) for housing each month. Also provided each year are a research grant of up to 1.5 Myen, insurance fee, and 58 kyen travel expenses in Japan. A candidate with experience in EPR of solids is highly preferred. Interested candidates please apply as soon as possible to Hideo Hosono, Project Leader of HOSONO Transparent ElectroActive Materials Team, Exploratory Research for Advanced Technology (ERATO), Japan Science and Technology Corporation and Professor of Materials and Structures Laboratory, Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama 226-8503, JAPAN; ☎: 81-45-924-5359; Fax: 81-45-924-5339 or 5359; E-mail: hosono1@rlem.titech.ac.jp. For further information about the Hosono Lab, visit:

http://lucid.rlem.titech.ac.jp/~www/

for the graduate school, visit:

http://www.iem.titech.ac.jp/Research/hosono/hosono.html.

TWO POST-DOCTORAL POSITIONS OPEN at CORNELL

I currently have two openings for postdoctoral associates in my research group. The areas of research will include: 1) Biophysical Studies of Model and Biological Membranes and Dynamic Structure of Membrane Proteins by Modern ESR; 2) Far-Infrared ESR Studies of Molecular Dynamics in Liquid Crystals, Polymers, and Biological Systems; 3) Two-Dimensional Pulsed ESR Studies of Molecular Dynamics in Liquid Crystals, Polymers, and Biological Systems. Interested individuals should contact: Professor Jack H. Freed; B52 Baker Laboratory of Chemistry & Chemical Biology; Cornell University, Ithaca, NY 14853-1301; e-mail: jhf@msc.cornell.edu. Applicants should be prepared to furnish a complete CV and at least two letters of recommendation.

TWO GRADUATE STUDENT POSITIONS AVAILABLE at LEIDEN UNIVERSITY

The Department of Biophysics of Leiden University, The Netherlands, has two graduate student (PhD) positions open for (bio)physicists or physical chemists who are interested in applying various magnetic resonance techniques for unravelling the fundamental molecular mechanisms of solar energy conversion in plant photosynthesis.

The Magnetic Resonance Group of the department has a longstanding tradition of applying sophisticated electron paramagnetic resonance methods to obtain information on the structure and function of the photosynthetic apparatus that cannot be obtained by other methods. The techniques comprise state-of-the-art time-resolved flash photolysis EPR equipment at a number of microwave frequencies ranging from 2 to 130 GHz, pulsed EPR, including 1D and 2D Electron Spin Echo Envelope Modulation (ESEEM) and pulsed Electron-Nuclear Double Resonance (ENDOR) spectroscopy, optically detected magnetic resonance (ODMR), and magnetophotoselection experiments, all at variable temperatures down to 1.2 kelvin. Several of the experimental set-ups have been developed in our own laboratory.

The first project involves the investigation of spin-isotope-labelled tyrosine and quinone cofactors of so-called Photosystem II of plants with a variety of EPR methods, including 1D and 2D ESEEM, pulsed ENDOR and time-resolved EPR at various frequencies in the range 2-130 GHz.

The second project involves the development and implementation of a new ODMR spectroscopy, in which changes in the circular dichroism of the photosynthetic preparation are measured and correlated with the detailed structure of the cofactors and their protein environment.

The two projects represent two different approaches aiming at understanding the mechanisms of photosynthetic energy conversion in sufficient detail to make it possible to develop environment-friendly biomimetic solar energy cells that harvest sunlight and convert it into sustainable chemical and electrical energy. The projects are embedded in a TMR Network of the European Union, comprising groups in Athens, Berlin, London, Munich, Oxford, Padova and Paris, which coordinates the investigations aimed at developing a source of sustainable energy.

The positions offered are each for a four-year term, and can be occupied as of now. Gross salary will start at 2374 Dutch Guilders/month plus DG 700/month special allowance, with yearly increases to DG 4037/month in the fourth year. Candidates should preferably have some experience with EPR or related spectroscopies. Experience in photosynthesis research is appreciated but not necessary. They should submit a full resumé, including a list of papers and practical works, and name and addresses (with phone, fax and email) of at least two referents.

Further information about the Magnetic Resonance Group can be found at the website of the Biophysics Department, with a description of current research and a list of recent papers: http://www.biophys.leidenuniv.nl/research/RCs/

For more information on the two projects contact Prof. Dr. A.J. Hoff, phone +31-71-5275955, fax +31-71-5275819, email hoff@biophys.leidenuniv.nl or Dr. P. Gast, phone +31-71-5275979, email gast@biophys.leidenuniv.nl. Applications should be sent to Prof. Dr. A.J. Hoff, Biophysics Department, Huygens Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands.

EQUIPMENT & SUPPLIES EXCHANGE

FOR SALE: VARIAN E12 SPECTROMETER

We have a Varian E12 spectrometer, of which the manual part is in good working order, which we would sell for a very nominal price. Enquiries can be directed to: Brian Hasinoff, Univ. Manitoba, Faculty of Pharmacy, Winnipeg, Manitoba, ☎: 1-204-474-8325; FAX: 1-204-474-7617; E-mail: b_hasinoff@umanitoba.ca

FOR SALE: VARIAN E-102 X-BAND BRIDGE

Varian E-102 X-band microwave bridge, with reference arm, fully checked and refurbished, recently replaced klystron with weak pitch S/N test included. Minimum price: US$5,000. To make an offer, contact Vanni Piccinotti, NMR Technical Services, Via del Berignolo 5, 50141 Firenze, Italy. ☎/FAX: 39-055-434841; e-mail: vpnmr@ats.it.

EPR INSTRUMENT WANTED

Searching for an EPR instrument in good working condition with variable temperature attachments. Contact Dr. Horia Caldararu, Romanian Academy, Institute of Physical Chemistry "I.G. Murgulescu," 77208 Bucharest, Romania, FAX: 40-1-3121147; E-mail: hcaldararu@chimfiz.icf.ro or hcaldararu@pcnet.pcnet.ro.

WANTED: USED BRUKER or VARIAN MAGNET

We are looking for a used Bruker or Varian magnet (with or without power supply). If you (or someone you know) have one which is sitting there collecting dust, please let me know. We will be happy to have it for a reasonable price. Please contact Dr. Jim Liu, Univ. New Mexico, College of Pharmacy, 2502 Marble NE, Albuquerque, NM, 87131; ☎: 1-505-272-9546; FAX: 1-505-272-6749; E-mail: jliu@unm.edu.

FOR SALE: SPECTRANOVA TEST EQUIPMENT

Test Equipment for sale: Brand New SpectraNova EPR spectrometer, test equipment from the manufacturer is for sale at reduced price. (Technical details may be seen on www.http://members.eunet.at/dr.-kondor). For more

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

information contact please dr. L. Kondor, fax + 43 1 877 8446, tel + 43 1 877 0553, E-mail: dr.-kondor@eunet.at

AVAILABLE: NITROXIDE RADICALS

A small collection of fairly well-preserved unique nitroxide radicals synthesized by Dr. L.A. Myshkina in the 1980's is now being made available:

- 2,6-bis(N-oxylo-tetramethyltetrahydropyrid-4-yl) thyophene
- 5-(N-oxylo-tetramethyltetrahydropyrid-4-yl) thyophene-2-al
- 2,6-dimethylenecyclohexanone substituted by 6-(N-oxylo-tetramethyltetrahydropyrid-4-yl) thyen-2-yl residues at both alpha-carbon atoms
- 4-chloro-4-nitro-TMP-N-oxyl

Small quantities of the following compounds are also available:

- 4-bromo-4-nitro-TMP-N-oxyl
- 1,4-di-TMP-butaine-bis-N-oxyl

For information about obtaining any of the above compounds, contact: A.E. Myshkin, Inst. Biochem. Phys., Russian Acad. Sci., Kosygin St. 4, 117977 Moscow V-344, Russia; E-mail: chembio@glas.apc.org.

FOR SALE: BRUKER ESP-300 RADIO-SPECTROMETER

The instrument is intended for investigation of materials by means of electronic paramagnetic resonance (EPR). It was purchased from Bruker Analytische Messtechnik GMBH by St. Peterburg quartz-glass factory "Stekvar" in 1989 and was installed in 1990 (tested in April 1990). But it was not used at all, because since that time this research activity was stopped at "Stekvar." It was not moved. Now the instrument is working completely. So, the instrument seems like new. This ESP-300 have maximum specification (for example, there is helium low temperature additional device provided by Oxford Instruments). This instrument is provided with system for double and triple resonance. There are some spare parts. System # is ZD 698. The instrument's technical details are: 1) it works in X-band (frequency: 9.79 GHz); 2) spare cavities: ER 4111VT, ER 4114 HT, ER 4105 DR; 3) NMR magnetometer is ER 035 M with ESR in cavity probe; 4) microwave bridge is ER 044 MRDH; 5) temperature range from 3.5 K (Oxford Instruments helium low temperature unit); 6) double & triple resonance system. For further information, contact Prof. Roman Eismont, E-mail: empire@peterlink.ru; ☎: 7-812-249-02-95; FAX: 7-812-249-51-14; Regular mail: 6 Shafirovsky Avenue, St. Petersburg 195273 Russia.

AVAILABLE: ISOTOPE-CONTAINING SPIN PROBES

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

FOR SALE - NMR MAGNETOMETER

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

WANTED: TERMINAL/MONITOR

Terminal/monitor for Bruker ECS 106 spectrometer wanted. Contact: Lon B. Knight, Jr., Furman University, Department of Chemistry, Greenville, SC 29613, USA; ☎: 1-864-294-3372; FAX: 1-864-294-3559; E-mail: lon.knight@furman.edu.

FOR SALE: VARIAN

Resonance Instruments has available:

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

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

NEED HELP in DESIGN and CONSTRUCTION of EPR ELECTRONICS?

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

AVAILABLE: TWO IBM 9000 COMPUTERS

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

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

AVAILABLE: USED VARIAN EPR EQUIPMENT

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

2) Varian ENDOR accessory, with Varian ENDOR cavity.

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

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

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

For details, contact James Anderson, Research Specialties, 5629 N. Maplewood, Chicago, IL, 60659, USA; ☎/FAX: 1-773-728-6570.