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Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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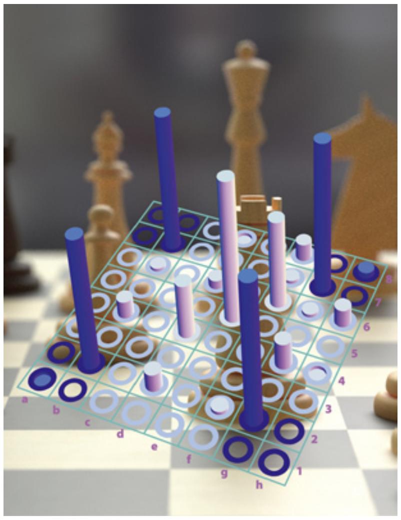

The cover picture illustrates some aspects of the research carried out by Michael Mehring, recipient of the Zavoisky Award 2008. It shows the density matrix tomography of an entangled state of a nuclear spin and an electron spin in $^{15}N@C_{60}$ (W. Scherer and M. Mehring, J. Chem. Phys. 128, 052305 (2008)).

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EasySpin 3.0

A major new version of EasySpin with many new features has been released. EasySpin is a free software package for spectrum simulation, fitting and data analysis in EPR to be used with Matlab, a scientific computation and visualization software that runs on Windows, Linux, and Mac.

EasySpin simulates single-crystal and powder cw EPR and ENDOR spectra of spin systems consisting of any number of electron and nuclear spins. Both matrix diagonalization and perturbation theory methods are implemented and offer a choice between high accuracy and fast performance. EPR spectra of nitroxides in the slow-motion regime can be computed and include an orthorhombic diffusion tensor, an ordering potential and the MOMD model. The new release also offers pulse EPR features: two-pulse and three-pulse ESEEM as well as HYSCORE spectra can be simulated. For this, EasySpin employs fast frequency-domain techniques. Interactive least-squares fitting of experimental spectra is another new feature. Available fitting methods include simplex, Levenberg-Marquardt, genetic and hybrid algorithms.

Visit www.easyspin.org for more information and for downloading the software.

Stefan Stoll
University of California, Davis

Editorial

Dear colleagues,

Yes, the International EPR/ESR Society is twenty years young. A young age for a society, the same as a young age for a human being, isn't it? I think now is a good time to take a look back, to analyze the present situation and to aspire to an even more prosperous future (please see Jack Freed's letter, the IES President, p. 3). The IES, on its 20th anniversary, deserves a comprehensive special issue of the *EPR newsletter* and it depends on all of us and our contributions to make this issue a success. It would be good in each, say, five or ten years flying by to recall this issue and to remember EPR and the IES in 2009 and enjoy the differences.

You are welcome to a tour in the DFT jungles for EPR spectroscopists, guided by Frank Neese, which Thomas Prisner arranged in his "Pro@Contra" column (p. 10). Stefan Stoll (see also 13/1-2, p. 9 and 24-26; 16/1, p. 21; and look to the left!) opens his "Software" column with an article by Gunnar Jeschke, 2009 Bruker Prize Lecturer, answering the question: "How reliable are broad distance distributions at a given signal-to-noise ratio and for given uncertainties on background corrections?" (p. 15). Our heartfelt congratulations to Gunnar! His long-standing collaboration with the EPR newsletter (see also 14/4, p. 14-16; 16/1, p. 15; 17/2-3, p. 8-9) is greatly appreciated.

A detailed report about the Zavoisky Award 2008 ceremony (p. 4) allows us to congratulate Michael Mehring on this highly deserved award. By the way, you may meet all Zavoisky Awardees, learn the true history of how the idea for this award was conceived, dive into the variety of applications of EPR, etc., if you order a book "Electron Paramagnetic Resonance: From Fundamental Research to Pioneering Applications & Zavoisky Award" edited by Kev Salikhov (p. 17). The "New Books and Journals" column also features a comprehensive overview of high-field EPR spectroscopy in biology and chemistry is given in a book by Klaus Möbius and Anton Savitsky. We are glad to share good news from Springer: the journal *Applied Magnetic Resonance* is offered to the members of the IES at about 12% of the regular list price.

Gus Maki, Bryn Mile, Brian Webster, Alessandro Bencini… a sad list of the names of our colleagues who left us. We share the pain of this loss with their friends and family and hope that our compassion and warm remembrances about these outstanding scientists may somewhat mitigate their pain. Our grateful memory will keep these people alive.

Laila Mosina

IES Annual Meeting

The 2009 IES Annual Meeting will be held during the ESR Symposium at the 51st Annual Rocky Mountain Conference which will be held in Snowmass, CO, USA from July 19 to July 23 in 2009.
The Annual Meeting timing has yet to be confirmed.
Please send any Agenda items to the
IES Secretary Prof. Sushil K. Misra
(skmisra@alcor.concordia.ca) as soon as possible.

Letter of the President

Dear Colleagues:

I am pleased and honored to serve as President of the International EPR/ESR Society (IES) for the next three years. During the 2008–2011 period I am joined by excellent Vice Presidents Michael Bowman (Americas), Thomas Prisner (Europe), and Michael Davies (Asia-Pacific), who will assist and advise me on the activities and policies of the IES. I would very much like to thank the former president, Wolfgang Lubitz, for his kind efforts in introducing me to the President's duties and for his dedication to and efforts on behalf of the IES. I would also like to thank Balaraman Kalyanaraman, Shozo Tero-Kubota, and Carlo Corvaja for all their contributions as Vice-Presidents these past three years.

As President, I am very pleased to have Sushil Misra as the IES Secretary in this very important position. He is grateful for the continued support and help from Shirley Fairhurst, the outgoing Secretary, in learning the many complex background tasks carried out by the Secretary. I am equally pleased that the role of Treasurer of the IES has been taken up by Tatyana Smirnova, who appreciates the help provided to her by the former Treasurer, Chris Felix.

The principal mode of communication within the IES and with the international scientific community is the *EPR Newsletter*. Laila Mosina has been the very dedicated Chief Editor since 2003, and we are very appreciative of the fact that she shall continue to edit and publish our *Newsletter*, maintaining it as the Society's main source of information. On behalf of the IES, I wish to express our gratitude to Laila and her Associate Editors, Candice Klug, Thomas Prisner, and Hitoshi Ohta, and Technical Editor, Sergei Akhmin, for their outstanding efforts at producing the excellent *Newsletter* issues.

It is a particular pleasure for me to preside over the IES this year, as it marks its 20th anniversary. Over these past 20 years we have witnessed a renaissance of the ESR/EPR field similar to what propelled NMR in prior decades into its current prominence. With new instrumental and theoretical technologies, the potential of EPR is now being realized in a wide range of scientific fields. As we in EPR know, this potential is exemplified by its high spin sensitivity, its excellent spectral resolution, its heightened sensitivity to the motion of the molecules, its ability to measure both short and long distances within and between molecules, its ability to provide medical images as well as microscopy of probe molecules with resolution down to micron dimensions, the limited degree to which the measurement disrupts the host, the availability of spin labels for a great variety of purposes, and the convenience of the measurement. In many ways EPR provides an optimal combination of all these features compared to other methods. These capabilities are valuable in both chemical and biological applications including the study of free radicals, metalloenzymes and organo-metallic compounds, polymers, protein and membrane structure and dynamics, molecular dynamics in complex fluids, electron transfer reactions, and spin-trapping. In the physics/materials field, new applications such as superparamagnetism, quantum dots, and quantum computing have emerged and add to studies of ferromagnetism, semi-conductors, and defect centers. Surely, the reader will be able to add to this extensive list.

The IES has, over the last 20 years, provided encouragement to these and other EPR developments worldwide in all scientific fields where it is employed, and aided in the dissemination of new ideas and methods in EPR spectroscopy throughout the scientific community. The IES will continue to actively support and participate in the numerous national and international conferences and workshops and encourage new, and support established, EPR groups and centers. It is my particular desire to maintain, and to re-establish where needed, ties amongst these EPR activities in a true international spirit. The IES will continue to foster its accessibility to its members, providing them with the latest information on the many activities in the field of EPR.

On the occasion of the 20th anniversary of the IES, I invite all the past IES Presidents, Executives, and IES Medalists to contribute their thoughts on the IES and its role in promoting EPR/ESR for a Special 20th Anniversary Issue of the *EPR Newsletter*. Let us all celebrate this momentous event!

Jack Freed

The Zavoisky Award 2008 to Michael Mehring

The 2008 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was awarded to Professor Michael Mehring, Stuttgart University, Stuttgart, Germany, in a ceremony marking his outstanding contribution to the pulsed ENDOR technique and concepts of quantum computing with electron and nuclear spins.

The ceremony was preceded by the Annual Workshop "Modern Development of Magnetic Resonance", 30 September – 3 October 2008.

The Zavoisky Award was presented on October 3, 2008 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 1500 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 AMPERE Society and the International EPR Society. The Award Selection Committee consisted of well-known experts in EPR: Professors G. Feher (La Jolla), D. Gatteschi (Florence), H.M. McConnell (Stanford), K. A. McLauchlan (Oxford), K. Möbius (Berlin), and the Chairman, K. M. Salikhov (Kazan). The selection of the Awardee was made after consultations with the Advisory Award Committee which comprises Yu. N. Molin (Novosibirsk), and Yu. D. Tsvetkov (Novosibirsk).

From left to right: A. M. Mazgarov, M. Mehring, S. Mehring, and K. M. Salikhov at the monument to E. K. Zavoisky.

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), J. H. Freed (1998), J. H. van der Waals (1999), H. M. McConnell and Bruker Analytik GmbH (2000), K. A. McLauchlan (2001), W. Lubitz (2002), W. L. Hubbell (2003), K. M. Salikhov and D. Stehlik (2004), H. M. Swartz (2005), J. Schmidt (2006), and Brian M. Hoffman (2007).

The selection of Professor Michael Mehring was made from many nominations solicited from international experts in EPR.

The Award 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 N. M. Valeev, the Minister of Education and Science of the Republic of Tatarstan. Professor M. Kh. Salakhov, Rector of the Kazan State University, Professor A. M. Mazgarov, President of the Tatarstan Academy of Sciences, Professor T. Prisner, Vice-President of the International EPR Society, and Dr. G. V. Stinsky, General Scientific Secretary of the Presidium of the Kazan Scientific Center of the Russian Academy of Sciences, warmly congratulated the laureate. Letters of congratulations from Academician V. A. Matveev, Academician-Secretary of the Department of Physical Sciences of the Russian Academy of Sciences, Professor W. Lubitz, President of the International EPR Society, Professor B. H. Meier, President of the AMPERE Society, Professor P. Callaghan, President of ISMAR, and Professor R. Bittl, Chairman of the Collaborative Research Center 498 of the Deutsche Forschungsgemeinschaft, were handed to Professor Michael Mehring.

A concert by a string quartet preceded and followed the ceremony. The event was concluded with a Banquet in honor of Professor Michael Mehring and his outstanding contributions to EPR. During their stay in Kazan the laureate and his spouse visited the museum of history of the Kazan State University and places of historical and cultural interest in Kazan.

The Organizing Committee owes special thanks to the Russian Academy of Sciences and Russian Foundation for Basic Research. ●

The Bruker Prize 2009

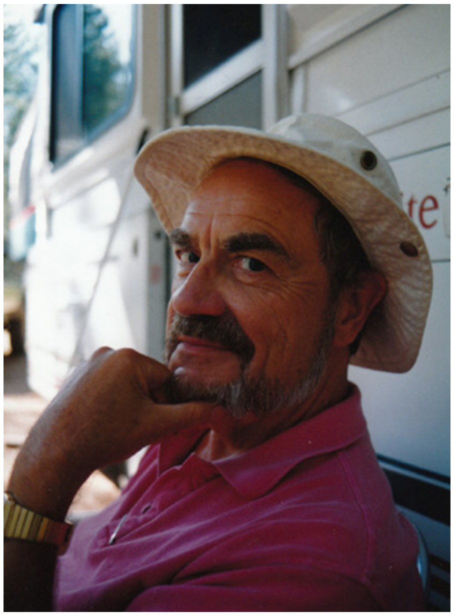
Gunnar Jeschke

**ETH, Zurich
Switzerland**

Gus Maki (1930–2008)

August (Gus) Maki was born in Brooklyn, NY, in 1930. His Finnish parents returned briefly to Finland with young Gus when he was a toddler (from this time he probably retained his strong liking of collecting mushrooms, including the frightening but delicious parasol mushrooms, that he disclosed to us during his visits to Berlin in the 1970s), but Gus mostly grew up in New York. He attended Brooklyn Technical High School, and after graduating in 1948, Gus enrolled at Columbia University, where he received his A. B. degree in Chemistry in 1952. He then began work on his Chemistry PhD at the University of California, Berkeley. The U.S. government had different plans for Gus at this time however, which resulted in a two-year stint in the U.S. Army, spent mostly stationed in Europe. During this time he learned more important things to do than to shoulder arms, for example to develop a fondness of French cuisine including a good red Bordeaux.

Upon returning to Berkeley in 1955, Gus decided to join the research group of a new assistant professor, Bruce McGarvey, using the relatively new technique of EPR spectroscopy to probe the details of metal ligand bonding in transition metal complexes. Gus was attracted to McGarvey's group by the promise of using EPR to directly probe the electronic structure of such molecules via the hyperfine and quadrupolar couplings. Their primary publication on this work (A. H. Maki, B. R. McGarvey, *J. Chem. Phys.* 29 (1958) 31), focusing on the EPR properties of copper(II) bis-acetylacetonate, is a classic in the field of EPR spectroscopy of transition metal complexes. In 1982 this paper was selected as a "citation classic", and in the associated article Gus explained that the paper had generated a great deal of interest because it was only at this time that chemists were really moving into using EPR, in part because commercial EPR spectrometers were becoming available, and their paper provided a chemist-accessible link between EPR parameters and molecular orbital theory and bond covalency.



Gus received his Ph.D. from Berkeley in 1957, and then moved to Harvard University, first as an Instructor of Chemistry (1957–1960) and then as an Assistant Professor (1960–1964). Gus continued to apply EPR spectroscopy to chemical systems in these years. In an *EPR newsletter* remembrance (see *EPR newsletter* 2004, vol. 14, no. 3, p. 13), Gus recalled that at that time the Harvard Physics Department was extremely powerful in magnetism and magnetic resonance research (with Purcell, Pound, Ramsey, Bloembergen and van Vleck), while the Chemistry Department had Assistant Professor August Maki. Gus started at Harvard before "startup funds" were the norm, but fortunately this was the immediate post-Sputnik era, so he was able to obtain NSF funding to assemble a homebuilt EPR spectrometer. "The Times They Are a-Changin": When R.D.B. was struggling to put together his first UC-Davis NIH proposal, 25 dense pages and all, Gus was proud to show him this first NSF proposal, which was in essence a letter to the NSF director explaining that he is a new assistant professor at Harvard, and he would like to explore applying EPR to chemical systems, so he needs money to build a spectrometer.

One of the chemical directions Gus pursued at Harvard was to generate solution radicals electrochemically inside the EPR cavity, work done in collaboration with his colleague David Geske. This opened a rich area of research, with new highly resolved radical spectra to measure and interpret, and a large number of Gus' Harvard EPR papers resulted from this technical advance. These experiments gave electrochemists direct new insights into radical formation and characterization, and this became a very active EPR research area for a number of groups following Gus' pioneering efforts.

Gus also continued to study paramagnetic inorganic coordination complexes. Most famously, he teamed with Dick Holm and Alan Davison to use EPR to study the d^7 Ni(III) ion in a bis-dithiolate coordinated complex. Gus' EPR spectra showed this to be a low-spin complex with significant spin density in a Ni d(pi) orbital, but also with significant delocalization into the ligand pi-system. This was a very different electronic structure picture than one promoted by Professor Harry Gray, who favored a purely ligand-radical description for this complex. A number of articles were published by both groups, and in his *EPR newsletter* reminiscence, Gus describes the experience of being caught up between the "Gray forces and the Holm forces".

Also it was at Harvard that Gus began his studies on photoexcited triplet states, later to be one of his major scientific targets via the optically detected magnetic resonance (ODMR) method. Gus was inspired by Hutchinson and Mangum's work on the naphthtalene triplet, and he and his student Jim Vincent quickly extended this work, using conventional EPR, to a number of other organic triplets photogenerated in durene host crystals.

At Harvard, Gus realized that Feher's new ENDOR technique could provide superior resolution and simplified analysis, not only for solid-state samples, but also for free radicals in liquid solution. The implementation of this idea occurred when Gus had a sabbatical semester in 1963, during which he was invited to spend a visiting professorship at Varian Associates in Palo Alto. This allowed him to work with Jim Hyde in modifying a cylindrical Varian cavity for high-power ENDOR, and they then applied this to the study of the proton ENDOR of Coppinger's radical in liquid n-heptane. Their first short communication (J. S. Hyde, A. H. Maki, *J. Chem. Phys.* 40 (1964) 3117) became another citation classic signaling the beginning of a new research era, ENDOR-in-solution. Hyde refined the instrumentation after Gus returned to teach at Harvard, and this became Varian's commercial ENDOR accessory to their EPR instrument line.

Despite his enormous successes in applying EPR to chemical systems, it was understood that the Harvard assistant professorships in those days were terminal appointments. In 1964 Gus moved out west

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to the University of California, Riverside, starting as an Associate Professor, followed by a promotion to Full Professor in 1968. Gus wanted to continue work on radical ENDOR, so he set up an ENDOR spectrometer at Riverside, not relying, however, on Varian Associates but rather on a collection of surplus instruments. Robert Allendoerfer assisted him as a postdoc in this endeavor and, ultimately, they succeeded in obtaining well-resolved ENDOR spectra of radicals in solution. They developed a phenomenological theory to describe the dependence of the ENDOR enhancement factor on key parameters of the radical molecule and solvent environment, which determine the delicate balance of the electron and nuclear relaxation rates necessary to obtain cw ENDOR signals.

To learn from the experience Gus Maki had accumulated already on ENDOR in solution at UC Riverside and to benefit from it for his own, still new high-power ENDOR efforts, K.M. spent a postdoctoral year 1969/1970 in his laboratory. There he met Maki's postdocs Brian Moores and Hans van Willigen. Together they shared the fun and frustration to rebuild the dismantled ENDOR spectrometer which had been cannibalized after Robert Allendoerfer had left the Maki lab. Eventually, they found a solution to the stray pick-up problems originating in the high-power radio frequency (rf) circuitry by properly grounding the dubious surplus devices and by impedance matching the ENDOR coil through incorporating a California wine bottle (empty) wrapped with a few turns of heavy copper wire (see A. H. Maki in *EPR newsletter* 2004, vol. 14, no. 3, p. 13). This resort to empty (and full) wine bottles enabled them to get through their day and night struggles with the beast of a machine and to perform an ENDOR study on the lifting of orbital degeneracy in high-symmetry large organic molecules by weak methyl-substituent induced perturbations. Gus was relieved when, after so many months of trials and tribulations with only noise recordings, finally beautiful ENDOR signals were creeping out of the noise floor. Then he shared the California wine celebration of the resurrection of the ENDOR machine with us, as did the other postdoctoral fellows in the Maki lab, Luis Alcacer and Chris Winscom. They were involved in Gus' other magnetic resonance activities, Chris Winscom for example in ODMR at zero magnetic field.

In 1967, Gus' successor in EPR at Harvard, Al Kwiram, used field-swept ODMR to study phosphorescent triplet states. The following year Jan Schmidt and Joan van der Waals from Leiden University reported triplet ODMR spectra at zero field using a microwave frequency scan supported by a slow-wave helix. Gus was impressed by this development, and this led to a discussion at an Asilomar Spectroscopy meeting with Mostafa El-Sayed of UCLA and Charles Harris of UCB. The group agreed to pool equipment resources and expertise in order to add ODMR capabilities to a phosphorescence spectrometer in El-Sayed's lab. Dino Tinti, Gus's future UC Davis colleague, was a postdoc in El-Sayed's lab at the time, and together this group of four used the instrument to measure the zero-field ODMR of individual vibronic bands of the 2,3-dichloroquinoxaline triplet. It was around July 1969, when Harris, Tinti, El-Sayed and Maki (*Chem. Phys. Lett.* 4 (1969) 409) sub-

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In Memoriam

Brynmor (Bryn) Mile (1936–2008)

Bryn attended Ruabon Grammar School in North Wales. He studied chemistry at Birmingham University where he obtained a 1st Class Honours degree in 1954 and a PhD in 1960, the latter with John Major and J. C. Robb on gas phase reactions of methylene. He then held a Post Doctoral Fellowship with Professor Fred Dainton at Leeds University for a year, where he worked on reactions of metal ions with free radicals in solution. He was appointed at Shell Research Ltd., in Thornton, by Maurice Sugden and worked with Alun Thomas and John Bennett on ESR studies of reactive radicals such as phenyl, isolated in cryogenic matrices formed using the rotating cryostat. He did additional work on tribology and lubricant stability and,

whilst also in the employ of Shell, spent a year in Emeryville in California. He joined Liverpool Polytechnic (later John Moores University) in 1973 as Reader (taking the Shell ESR spectrometer with him and inaugurating a new field of research there, in collaboration with Harry Morris), and then moved to NRC in Ottawa, Canada in 1984, the year he was also awarded a DSc. While at NRC he worked in close collaboration with Tony Howard on reactions of metal atoms with organic and inorganic substrates using cryochemical techniques. He returned to the UK in 1990 to take up a position at the University of Wales in Cardiff. He left Cardiff in 1995 and accepted a visiting position at Bristol University, to work with Peter Timms on metal atom chemistry.

Bryn was a proud and passionate Welshman, with many interests beyond chemistry. He served as a socialist councillor in conservative Chester, he was a painter and sculptor, and also a poet. Other activities included fly-fishing and a study of philosophy. His life was all the more remarkable considering the fact that he developed juvenile diabetes at the age of 10 and lived with it for 62 years, never letting it hold him back from what he wanted to do in life.

He was married to June who studied Social Science at Birmingham. They have two children: David, a GP in Newark and Sian, a former English professor at Augusta State University in Georgia and currently an aide to Julie Morgan MP. They also have four grandsons.

Tony Howard and Chris Rhodes

mitted their manuscript describing the novel optically detected ENDOR experiment in zero field on photoexcited 2,3-dichloroquinoxaline. Interestingly, independent work on the same subject was performed at the same time by the Leiden group (I. Y. Chan, J. Schmidt, J. H. van der Waals, *Chem. Phys. Lett.* 4 (1969) 269), and the results are in essential agreement with each other.

Based on this success, Gus constructed an ODMR instrument at Riverside, and he became so interested in the power of ODMR that he largely focused on this technique for the rest of his career. But also the way to building up zero-field ODMR and even extending it to ENDOR capability was a long and weary one. It needed the tenacity of Chris Winscom to eventually lead it to success. Like ENDOR-in-solution, also zero-field ODMR had rather sparse phase around 1969 as far as new results were concerned, and Gus turned out to be not too patient with his postdocs. He gave us all a hard time in the demanding discussions with him. And robust, but scientifically sound responses to his criticisms were needed in this very provocative period to convince him that we were indeed on the right way to solve the instrumental problems. But when both ODMR and ENDOR-in-solution were rolling, Gus kept company with us in some long nights in an effort to cheer us up to get first signals before the coolants ran out. Rather frequently, such nights ended in Frank's bar in downtown Riverside for a game of pool, a beer and a bowl of chili. And even the animating dancing activities next to us could not stop our heated discussions about science, society, and the Vietnam War.

Shortly later, Gus realized that in addition to examining small organic molecules, zero-field ODMR would have the sensitivity and resolution to be useful for examining photo-induced triplets in non-crystalline biological molecules such as DNA constituents. At Riverside, he and his group, among them Joseph Zuclich, demonstrated the promise of this technique both with protein and nucleic acid samples. This was the research area where a string of German postdocs got consecutively involved in the early 70s: Dieter Schweitzer,

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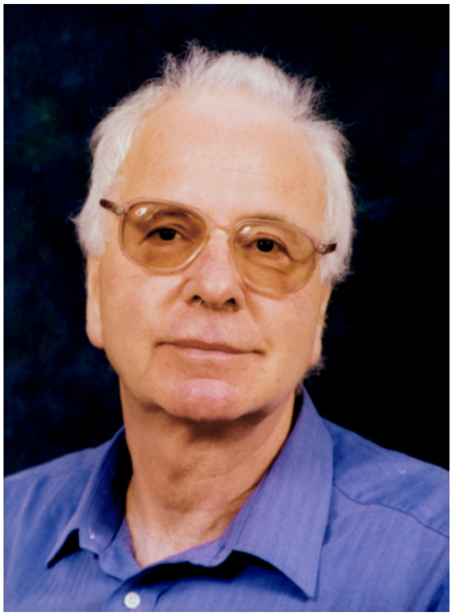
In Memoriam

Brian Webster (1939–2008)

Brian Webster was born in Bournemouth on the 20th June 1939. He was a spirited boy, enjoying climbing trees at the nearby recreation ground. After passing the 11-plus he attended Bournemouth Grammar. As well as playing rugby and football (in goal since he was tall) he enjoyed athletics and threw the discus for Hampshire. He learnt the piano at an early age and continued playing throughout his life.

He went up to Magdalen College Oxford to study Chemistry in 1958, spending his final year on a theoretical chemistry project with Professor Coulson in the Applied Mathematics department. During one of his holidays he met his future wife Mary who was studying physics in London.

Brian and Mary were married in Bournemouth in 1961, spending their honeymoon travelling around Scandinavia taking in the culture and scenery. After a year in Oxford they sailed to Australia via Suez, under a Commonwealth Scholarship. They returned via the Panama Canal to Glasgow. Brian secured an assistant lecturer post at Glasgow University whilst he completed his PhD in theoretical chemistry. He was then appointed to a permanent lectureship at Glasgow University.



His four children, Bridget, Adrian, Sonia and Zuleika were born between 1964 and 1970. In 1972 the Webster's took a one-year sabbatical leave at the University of Stuttgart in Germany – appreciating a different culture and language.

At Glasgow University his area of research was theoretical chemistry. He was considered a superb lecturer, ranging from introductory chemistry courses to advanced bonding and quantum mechanics. His research students found his wide knowledge – outside chemistry – stimulating.

He was internationally known for his work on bonding, solvated electrons, muons and other topics, attending and speaking at scientific meetings and conferences. He made visits to other universities including a short term professorship at the university of Paris. He co-edited the book Electron-solvent and anion-solvent interactions, published in 1976, which described the current state of research on solvated electrons. His book, Chemical Bonding Theory, was published in 1990, and was also translated into Japanese.

In Autumn 2000 he retired and was designated an Honorary Research Fellow. He continued pursuing his own research from home including academic writing.

His wide range of interests included music – he played the piano, the clarsach harp and had an appreciation and knowledge of both classical and modern music. He was widely versed in the arts – painting, sculpture and literature. He loved walking, both in Scotland and the Alps, and mountain biking in the Highlands. He enjoyed gardening with a love of flowers both in his own garden, and in gardens throughout Europe.

Those involved in muonium chemistry owe Brian a great debt for putting the subject on a firm footing with what must have been amongst the first – if not the first – computational backing: Born Oppenheimer checks, ab initio structure determinations of muonium-containing radicals etc. He is remembered too for his stentorian voice and inimitable chairmanship style! My own memory of Brian is of a generous and kind man, who was a wonderful source of humanistic support and intellectual succour, particularly to the young.

He died on 17 October 2008 and is survived by his wife, Mary, his four children and five grandchildren.

Chris Rhodes

Jost von Schuetz (still in Riverside) and Peter Dinse (already in Davis). They did not only contribute to push the new biological ODMR projects into the publication phase but they also turned out to be expert craftsmen for the various phases of completion of Gus' mountain cabin.

In 1974, in one of the State of California's cyclic economic downturns, the UC powers decided that they needed to downsize the UC Riverside campus. Interestingly enough, other campuses were offered the option of recruiting key Riverside faculty, an interesting distillation process indeed. UC Davis was fortunate enough to move Gus Maki up to Davis, where he was to remain for the rest of his career. At Davis, Gus largely focused on the further technological development of the ODMR technique and its concomitant application to the study of increasing complex and interesting biomolecules. He was able to establish an NIH funded program studying protein – nucleic acid interactions via photo-induced triplet state ODMR, including the effects of antibiotics in affecting such interactions. In his time at UC Davis, Gus was always a key member of the faculty, and a driving force for a strong physical chemistry division and high standards across the board. He trained several generations of students, both undergraduate and graduate, with these high standards. Gus was part of a very strong UC Davis magnetic resonance group, along with Gerd LaMar, Dino Tinti, and Nancy True, and his presence here was crucial for later bringing Matt Augustine and David Britt to the department. Gus was a great mentor to his new junior magnetic resonance colleagues. We could always count on him for great advice in magnetic resonance, physical chemistry, or practical things from equipment construction to grant writing. Plus he always was happy to convey a refreshingly cynical view of the campus administration! And his former postdocs will certainly share Chris Winscom's remembrance that "Gus was good fun if you could handle a more robust line of conversation, and he enjoyed engaging in quite challenging and provocative scientific discussions around magnetic resonance. He was open to the more imaginative proposals if they offered something new to be found out. We learnt a lot from him".

Gus formally retired in 1994, but maintained an active NIH-funded ODMR focused laboratory for a number of years after

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In Memoriam

Alessandro Bencini (1951–2008)

Alessandro Bencini, Professor of Inorganic Chemistry at the University of Florence, Italy, died on July 21, 2008 at the age of 57. He was born on April 18, 1951 in Fauglia, a small town not far from Pisa, in Italy. As was usual at that time he attended the Liceo Classico, the high school for brightest students, for 8 years, where he studied Latin and 5 years Greek, much Philosophy, and some Mathematics. Chemistry was essentially not on the syllabus. He went on to study Chemistry in the University of Florence, where he graduated in 1975 with a thesis on the electronic spectra of transition metal complexes in low-symmetry environment. The degree was Laurea, which required five years of studies after Liceo. It is worth noting that in Italy there was no PhD degree until the 1980s. After a short period as a school-teacher he obtained a position as a researcher in the Florence CNR Laboratory where he remained until 1987, when he moved to the University of Florence, first as an associate professor and then as a full professor.

For his thesis Alessandro worked with Ivano Bertini, who was being promoted to a full professor just at that time, and with me, at that time a young assistant of Professor Sacconi. The interest of the Lab was in the electronic structure of paramagnetic transition metal complexes in low-symmetry environments. The choice of EPR as a sensitive local probe to look into the metal ion coordination environment was a very appropriate one and we moved energetically in this field for which no previous expertise was available in Florence. Alessandro played a key role in the development of EPR in Florence, aided by the fact that he had an excellent theoretical background, which allowed him to follow the quantum mechanical subtleties associated with the interpretation of the spectra. But he was also an excellent experimentalist and therefore played a major role in the implementation of the liquid helium attachment. Again, it was terra incognita: the helium dewar came from Milan by truck, and all the previous expertise in Florence was in the use of liquid nitrogen for magnetic measurements. We spent a few nights trying to fix all the leaks, and it was Alessandro who finally succeeded in measuring the first low-temperature spectra.

Above Abragam and Bleaney's book, he highly appreciated the elegant book by Griffith. He was fascinated by the extensive use of group theory, which was needed for somebody who was interested in low-symmetry systems. One of the great themes of his scientific life was the use of the spin Hamiltonian, which attracted him by its relative simplicity in the characterization of the spectra and for its correlation with the basic structural parameters. His first paper was on the calculation of ligand field spin-orbit parameters in five-coordinated complexes, and the last is entitled "Some considerations on the proper use of computational tools in transition metal chemistry", where his critical and rigorous attitude is clearly expressed.

Conceptually simple as it is, the spin Hamiltonian approach gives rise to many difficulties when the **g**, **A**, **D**, etc. tensors must be compared with calculated ones. He developed a general program in which the energy levels of the relevant system are calculated within the ligand field approach and the spin Hamiltonian parameters are calcuhis retirement. He and his wife Judy also spent a good deal of time in these retirement years up at their beloved Mt Lassen cabin (where the shown picture of Gus was taken), and time with their family, including new grandchildren, was a source of great joy.

Gus Maki earned a number of honors during his career. As a graduate student, he was the Allied Chemical and Dye Fellow (1956–1957). As mentioned earlier, in 1963–1964 he was a Visiting Professor at Varian Associates. He was a Guggenheim Fellow in 1970–1971, which allowed him to spend a year at the Physics Institute of the University of Stuttgart. He was a Visiting Professor at the Free University of Berlin in the Spring of 1981, and at the Department of Biology at Johns Hopkins University in Spring 1985. He was selected as the Chevron Lecturer in the Department of Chemistry at the University of Nevada, Reno in 1983. In 2000 he was elected as a fellow to the International EPR Society.

Gus Maki passed away on October 22, 2008. He had fought hard against several cancers over past few years, and ultimately succumbed to a pulmonary embolism. He is survived by his wife Judy Maki in Davis, his children Paul Maki and Linda Maki (Menlo Park CA), Jeff Maki and Ian Maki (Seattle WA), and stepchildren Michael Schulman (Sacramento CA) and Apryl Murray (Las Vegas NV), along with six, soon to be seven, grandchildren.

Gus was always a real gentleman, and one of the nicest and most stimulating fellows one would ever meet. He will be greatly missed by his family and friends and by the magnetic resonance community as a whole. In his memory the Chemistry Department has established a Gus Maki Memorial Fund to support physical chemistry graduate students. Contributions to this fund can be mailed to Chairman Carlito Lebrilla, Department of Chemistry, UC Davis, 1 Shields Ave, Davis CA 95616. (Checks can be made payable to the "UC Regents" with a note on the memo line that the contribution is for the Gus Maki Fund.)

R. David Britt
(University of California at Davis),
Klaus Möbius
(Free University Berlin)

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lated through a projection technique, that allowed, in principle, for all orders.

Perhaps the most important results he obtained in this initial period were the correlations he established between structure and spin Hamiltonian parameters in five-coordinated complexes ranging from square pyramidal to trigonal bipyramidal. He was fascinated also by the exchange phenomena. He was particularly concerned with a mixed-valence dinuclear system which can be considered as the best model for double exchange, the driving force for colossal magnetoresistance in manganites. In his early career as an EPR spectroscopist he measured the single-crystal spectra, and returned to them in his time, as a theorist producing also new experimental data using high-frequency EPR.

His scientific interests moved to the use of theoretical models, more sophisticated than the ligand field treatments he used in the beginning, but the main reason was the need to calculate the spin Hamiltonian parameters. For example, he was one of the first scientists to use $X\alpha$ to calculate the parameters of tetrahedral copper(II) complexes, which were not correctly described by the ligand field. The next step was that of calculating the magnetic interaction in dinuclear copper(II) clusters, using the broken-symmetry $X\alpha$ approach, to pass to more complex clusters. By moving to the use of DFT, he returned to his favorite theme of mixed-valence compounds, but he also started to be interested in open-shell organic compounds. Recently he had become interested in more complex systems, such as magnetic molecules attached to gold surfaces. It is true to say that Alessandro did not like to follow the fashion, to coin a phrase. He wanted to tackle problems which allowed quantitative and unequivocal solutions.

A pure scientist who preferred understatement, Alessandro was a gentle person, but did his best to hide this under a rough appearance. He was a stimulating but uncompromising lecturer: if a complex equation was needed, no discount was made to the student. But he was able to charm them with a friendly attitude, perhaps going to a pub together. We had a lifelong collaboration and published together also a book on EPR of exchange coupled systems where his fingerprint of rigor is clearly visible. He was my first student but beyond that we were very good friends and his untimely death has been a great shock. We all miss his critical attitude and illuminating suggestions.

Dante Gatteschi

Density Functional Theory and EPR Spectroscopy: A Guided Tour

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Introduction

In recent years, the resolution of EPR spectroscopy has been steadily increasing owing to the advent of powerful pulse techniques and sophisticated high-field instruments. Consequently, a much larger amount of experimental data can be obtained on given system compared to the situation, say, twenty years ago. This fortunate situation immediately brings up the question of the interpretation of the data and calls for theoretical calculations. In fact, calculations are being used by most advanced EPR laboratories now in order to complement the data. The goals of theory are at least twofold: (1) *understanding* the molecular origin of the spin-Hamiltonian parameters in terms of the geometric and electronic structure of the system under investigation, (2) helping to *analyze* the experimental data.

Under (1) diverse aims may be envisioned that range from obtaining qualitative insight to sorting a number of candidate structures according to their likeliness of representing the real system. Under (2) the calculations are asked to provide a reasonable set of starting values for detailed EPR simulations. This is particularly pressing if hyperfine and quadrupole information on a large number of nuclei is present in the data. It is at least difficult and laborious if not frequently impossible to obtain the full information of the tensor principal values and their orientations from experiment alone or to correctly assign a given hyperfine pattern to a given group of nuclei in the system.

In all these cases, contemporary theory, if exercised with sufficient care, can be of invaluable help to the experimentalist. Indeed, compared to the complexity of using a modern high-tech spectrometer, it is relatively straightforward to learn how to do such calculations. After having spent some time in a theory group, motivated students will in many cases be able to successfully carry out the calculations themselves.

In this short note some practical aspects of the calculation of EPR parameters from 'first principles' are briefly touched. The recommendations reflect the author's experience over a period of about a decade and no attempt will be made to justify each statement in detail. The recommendations are, to some extent, subjective and it is fair to say that not all opinions voiced below are shared by all members of the community. Detailed reviews that cover most technical details have recently been published [1–4].

What can be calculated?

A number of modern day quantum chemistry programs (*vide infra*) can calculate hyperfine tensors, *g*-tensors, zero-field splitting tensors and quadrupole tensors to varying degree of accuracy. Relaxation times cannot yet be calculated and higher order terms in the spin-Hamiltonian have received only limited attention. Additional properties like the linear electric field effect can, in principle, be calculated relatively straightforwardly but presently there does not appear to be much interest in this quantity from the experimental community.

Which theory to use?

The theoretical framework for the vast majority of present day EPR calculations is provided by Kohn-Sham density functional theory (DFT) [5]. There are several reasons for this success, the most striking ones being that it is computationally efficient, easy to use and easy to interpret. Competing theories are based on correlated *ab initio* methods [6]. These are commonly believed to provide systematically higher accuracy than DFT but they are still restricted to rather small molecules owing to the high computational effort involved. Calculations using coupled-cluster (CC), the closely related quadratic configuration interaction (QCI) or the so-called multireference theories (MR-CI, CASPT2) belong to a specialist domain for probably at least some time to come. The computationally efficient unrestricted Hartree-Fock theory (UHF) or the complete active space self-consistent field theory (CASSCF) are not recommended and usually provide results that are significantly inferior to those obtained from DFT approaches[1] [7].

Which functionals to use?

There are many different density functionals upon which the calculations can be based. Some of these functionals even contain empirical parameters that can be adjusted to obtain better agreement with experiment. To some extent, this is an unfortunate situation since given the proliferation of density functionals in recent years, it becomes more and more difficult to judge the quality of a given study or to compare the results of different studies. The quantum chemistry community is usually quite strict in 'benchmarking' new theoretical methods in order to obtain the typical error bars of a given method for a given property [5]. While to some extent this is also being done for EPR spectroscopy, the majority of functional developers only benchmark total energies and perhaps molecular geometries. Fortunately, it turns out that the mainstream functionals are also suitable for EPR calculations. In the author's opinion, it is helpful to stick to a small number of standard functionals and accept their systematic shortcomings rather than to try to fit adjustable parameters to each and every property of each and every molecule of interest. In particular, this concerns the so-called fraction of Hartree-Fock (HF) exchange that is frequently fitted to experimental data: the 'optimal' fraction of HF exchange depends on the property of interest and the system of interest (radical or metal, oxidation state, spin-state etc.).

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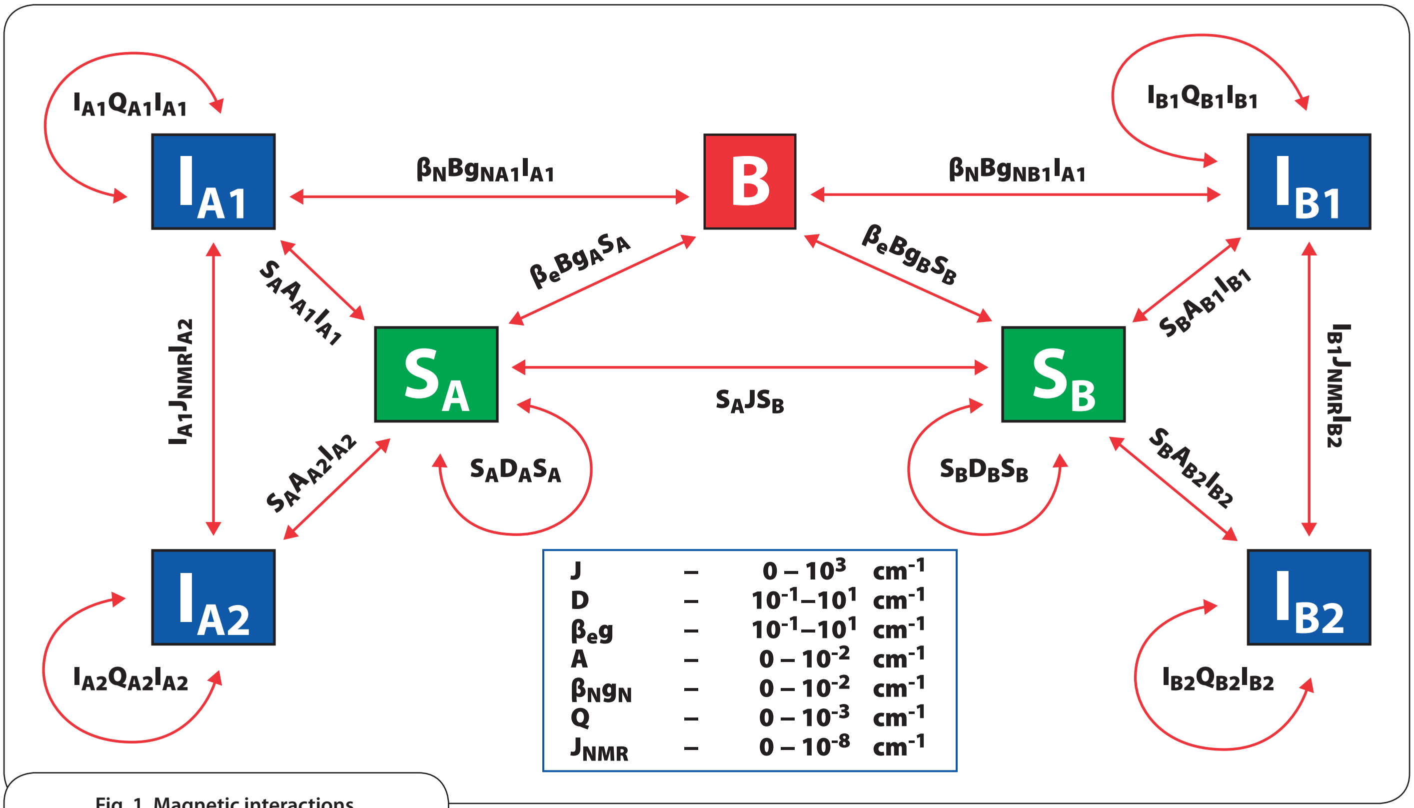
[1] The exception to this statement is the calculation of zero-field splittings where CASSCF based calculations can be significantly more successful than DFT approaches.



J	–	$0 - 10^3$	cm^{-1}
D	–	$10^{-1}–10^1$	cm^{-1}
$\beta_e g$	–	$10^{-1}–10^1$	cm^{-1}
A	–	$0 - 10^{-2}$	cm^{-1}
$\beta_N g_N$	–	$0 - 10^{-2}$	cm^{-1}
Q	–	$0 - 10^{-3}$	cm^{-1}
J_{NMR}	–	$0 - 10^{-8}$	cm^{-1}

Fig. 1. Magnetic interactions probed by EPR spectroscopy

With this in mind the following recommendations can be made: (1) all EPR calculations should be preceded by at least a partial optimization of the geometry of the system in order to obtain meaningful results. Such calculations are best done with a non-hybrid functional such as BP86, PBE or TPSS since in this case (given a good program) the extremely efficient 'density-fitting' approximation can (and should) be used. The time saved (compared to a hybrid DFT calculation) should then rather be invested in a better basis set or a more realistic model of the system of interest. (2) For the EPR property calculations all benchmark calculations have so far shown that, at least on average, hybrid DFT methods (e.g. those that involve a fraction of Hartree-Fock exchange) give better results than those delivered by the 'pure' functionals. Of the hybrid functionals the de-facto standard in chemistry is the B3LYP functional which also performs very well in theoretical EPR spectroscopy. Viable alternatives are the PBE0 and TPSSh functionals that are at least as reliable as B3LYP and sometimes even better [8]. In particular, there have been accumulating reports in the theoretical literature that B3LYP does not behave consistently for larger molecules (in terms of total energies) while PBE0 does [9, 10].

Which basis sets to use?

All DFT calculations have to be carried out in a finite set of auxiliary functions (the 'basis set') that is used to expand the Kohn-Sham orbitals. In the limit of a mathematically complete basis set, the results do only depend on the functional used and no longer on the particular choice of basis set. Hence, since the basis set is an 'artifact' of the theoretical procedure one should try to use basis sets that are large enough such that the deviations from the basis set limit are small. Studies with results that are dominated by basis set incompleteness effects are fundamentally uninteresting and do not reveal anything of interest about the system under study. Generally, in DFT the results converge rather fast with respect to the basis set size such that the basis set incompleteness issue is not overly pressing. Yet, one has to be somewhat careful since properties such as the isotropic hyperfine coupling have more stringent basis set requirements.

In general, the basis sets used in the geometry optimizations should be of at least polarized double-ζ but better of singly polarized triple-ζ quality. Particularly suitable basis sets of this type have been developed by Ahlrichs and co-workers (SVP and TZVP). These basis sets are better and more consistent than the popular Pople-style bases 6-31G(d,p) and 6-311G(d,p). For anions diffuse functions should be added. For results close to the basis set limit the calculations should employ three-sets of polarization functions, e.g. TZVPP which amounts to the use of 2d and 1f polarization function on each heavy element and 2p and 1d function on each hydrogen. Calculations with such basis sets are somewhat expensive but can still be done for large molecules with the most efficient contemporary program packages.

For the calculation of EPR properties similar basis sets can be used with a few exceptions: (a) on atoms for which the isotropic hyperfine coupling is to be computed the basis sets require additional flexibility in the core region. This can be achieved by either decontracting the standard basis sets (which requires some experience and experimentation) or by using predefined special basis sets. For the first row atoms, the decontractions reported by Barone (EPR-II and EPR-III) [11] work well (in the valence region these basis sets are roughly of SVP and TZVPP quality respectively). For the second row the IGLO-II, IGLO-III and IGLO-IV bases defined by Kutzelnigg and coworkers [12] for NMR calculations work well, while for first-row transition metals we have defined a set of bases that are called CP(PPP) [13] and that, so far, have given good results. (b) if there are heavier elements in the system (say, first transition row and heavier), relativistic effects should be included in the calculations. For geometry optimizations the leading relativistic effects can be treated by using 'effective-core potentials' (ECPs) that are implemented in most major program packages. However, these are not suitable for the calculation of EPR properties, in particular not for hyperfine calculations. Here, at least scalar relativistic all-electron calculations should be performed. Calculations based on the ZORA formalism have become somewhat popular and can, with suitable programs, now be performed as efficiently as nonrelativistic all-electron calculations (see below). For such calculations special relativistic basis sets have to be used [14].

Which programs to use?

A number of programs have been used for EPR property calculations. Some of them are commercial and some are not open to the general public. Below an attempt is made to provide a reasonably unbiased comparison.

Many programs are suitable for the geometry optimization part. The most popular program is without the Gaussian series of programs. Gaussian features a high-quality and very stable geometry optimization algorithm that is probably not surpassed by any other program. However, in particular for pure DFT calculations with density fitting, Gaussian is outperformed (in terms of execution time) by a number of other programs including TurboMole, Jaguar and ORCA.

The choice of software is more restricted when it comes to EPR property calculations. The Gaussian program has some functionality for hyperfine couplings and g-tensors. However, the former has so far been only available for $S = 1/2$ states, there is no spin-orbit correction to the hyperfine coupling and the g-tensor part uses a spin-orbit correction that is inferior to that used by other programs (vide infra).

The other commercial package that has significant EPR functionality is ADF which is essentially restricted to functionals without Hartree-Fock exchange. ADF has strong relativistic capabilities on the basis of the ZORA formalism and has been the first to derive and implement one- and two-component approaches [15, 16]. ADF computes the complete hyperfine tensors (although the spin-orbit correction and the Fermi contact term can not simultaneously be calculated and the procedure is restricted to $S = 1/2$) as well as *g*-tensors and quadrupole tensors but does not feature zero-field splittings. At least in our hands the results for *g*-tensor calculations are significantly inferior to those obtained with the most accurate approaches described below [17, 18] since (a) no hybrid functionals can be used and (b) the 'effective potential' spin-orbit operator used has certain shortcomings which are particularly apparent for light elements [19].

There are three academic programs that have significant EPR capabilities: Dalton, ORCA and MagRespect. Dalton is freely available and is particularly strong in the field of multiconfigurational SCF approaches [20, 21] to which many pioneering contributions have been made by its authors. Dalton bases its DFT theories on open-shell spin-restricted wavefunctions [22]. As far as is possible to judge from the literature, the results are similar to but perhaps slightly inferior to the results obtained with spin-unrestricted approaches with other programs. Dalton has been reported to calculate all parts of the hyperfine coupling (where the Fermi term is problematic for spin-restricted approaches) and the *g*-tensor. The ZFS-tensor has been implemented for CASSCF wavefunctions [23] but apparently not yet for DFT.

The MagRespect program by Malkin, Kaupp and co-workers has been reported to have many capabilities in theoretical EPR spectroscopy and features a wide range of different DFT approaches ranging from nonrelativistic and scalar-relativistic one-component to relativistic two-component methods [24–28]. It also features a number of nonstandard functionals [29, 30]. The program has been reported to calculate all parts of the hyperfine coupling, quadrupole splittings, the *g*-tensor and the spin-orbit contribution to the ZFS-tensor. The program does not seem to be publically available.

The ORCA program has been developed in our research group, is publically available and also features a wide range of theoretical methods ranging from highly correlated single- and multireference *ab initio* methods to DFT and even semi-empirical methods [7, 18, 31–40]. In terms of EPR spectroscopy, the program is perhaps presently the only one that features the full range of properties: all parts of the hyperfine and quadrupole coupling tensors, the *g*-tensor for any multiplicity as well as the spin-spin and spin-orbit contributions to the zero-field splitting. In particular for the latter a new method has recently been developed that rectifies some of the shortcomings of previous methods [39]. The program also features scalar relativistic corrections using the ZORA approach and special basis sets for such calculations have most recently been made available.

MagRespect, Dalton and ORCA all base the treatment of spin-orbit coupling on the spin-orbit mean-field approach developed by Hess, Marian and co-workers [41]. It is believed to provide a fairly rigorous and accurate approach to the full two-electron Breit-Pauli operator and has proven its accuracy in many applications. MagRespect and Dalton use Schimmelpfennig's AMFI code [42] to compute the SOC which makes two additional approximations which lead to a small, controlled loss of accuracy. These approximations are avoided in the ORCA program [19].

How long do you have to wait?

In principle, calculations can nowadays be carried out on pretty much any computer but most programs (excluding ORCA and Gaussian) are only available for Unix based platforms. The best way to run such calculations is on PC clusters, perhaps taking advantage of parallelization (however, massive parallelization is not supported by any of the programs mentioned above). Computing molecular geometries can be fairly laborious and may take several days of computer time. Calculations can be performed with up to roughly 100 to 200 atoms. They are best started from a good guess at the final geometries that can be obtained from X-ray crystallography, initial cheap force field calculations or from an earlier calculation for a closely related system.

Property calculations can be carried out for any system for which the geometry optimization was feasible. If one uses density fitting in the geometry optimization but a hybrid functional for the property calculation one should be prepared that the property calculation may take as long as the entire geometry optimization. Nevertheless, the property calculations rarely take more than 1–2 days of computer time except for rather large molecules.

What accuracy to expect?

Hyperfine Couplings. For hyperfine couplings of organic radicals DFT methods are often surprisingly good and can even compete with elaborate *ab initio* approaches at a small fraction of the computational cost. Practically all of the challenge is to compute the isotropic Fermi contact term since the dipolar hyperfine tensors are relatively straightforward to compute. If everything goes well, the residual error of 'primary' hyperfine couplings is about 10–20% [43]. With 'primary' one refers to those nuclei that are situated close to, or carry a significant amount of the spin density. 'Secondary' hyperfine couplings involve those nuclei that either sit in a node of the SOMOs or a more distant. Here, the

▶

errors are usually somewhat larger although many π-radicals are well described by DFT. For the very small (1–2 MHz) hyperfine couplings of distant nuclei many factors come into play, foremost the accuracy of the calculated spin-density distribution, the geometry, environmental effects among others. One should not be surprised to see errors on the order of a factor of two.

Very challenging for theory are the large hyperfine couplings of transition metal nuclei. Here it frequently happens that all three contributions (Fermi contact, dipolar and spin-orbit) are of about equal magnitude but of opposing signs. However, the physical origin and requirements of the three terms are very different: The Fermi contact term is dominated by the region around the core and depends critically on the core-level spin-polarization. This core polarization is considerably underestimated by DFT (up to a factor of two depending on the number of unpaired electrons). Increasing levels of HF exchange increase the spin polarization. At 100% HF exchange (e.g. the HF method itself) the core polarization is enormously overestimated. The dipolar part of the hyperfine interaction is primarily governed by the spin distribution in the valence shell and thus depends sensitively on the polarity of the metal-ligand bonds. In general, DFT tends to exaggerate the covalency of these bonds which results in too much spin on the ligands. This is particularly pronounced for non-hybrid functionals. Finally, the spin-orbit part is a response property and hence depends to a large extent on the quality of the excitation spectrum, in particular on the d-d transitions. These transition energies are often overestimated by DFT. Thus, the simultaneous underestimation of the core-polarization, underestimation of metal spin-population and overestimation of transition energies leads to calculated metal hyperfine couplings that can be significantly in error. It is readily appreciated how difficult it is to develop theoretical methods that treat all three contributions equally well. Yet, the trends are usually well represented by DFT methods and following proper calibration it can be a useful tool even for transition metal EPR.

***g*-Tensors.** The *g*-tensors of organic radicals are often calculated with excellent accuracy with DFT methods. Using the best combination (hybrid functional, spin-orbit mean-field operator and sufficiently large basis set) many *g*-tensors have been calculated within 100–200 ppm of the experimental values. Exceptions with large errors do, however, occur – the H_2O^+ and OOH radicals are cases were the DFT errors amount to a few thousand ppm.

Again, for transition metal complexes, the situation is much more difficult. The *g*-shifts are up to a thousand times larger and – being a response property – the same comments apply as for the spin-orbit contribution to the hyperfine coupling. In the worst cases, for example many Cu(II) complexes, an underestimation of up to a factor of two is observed. Again, the trends are reasonable and more reliable than the absolute values.

Zero-Field Splittings. The ZFSs of organic triplets, diradicals and carbenes are dominated by the direct spin-spin part [40]. DFT has been very successful for the calculation of this contribution. However, for unknown reasons this requires a spin-restricted treatment and even modest amounts of spin polarization immediately deteriorate the agreement with experiment. For heavier main group elements, the spin-orbit coupling contributions become dominant. Only very recently has the correct response formalism been developed which allows a calculation of these terms on the basis of DFT [39]. The results have been fairly reasonable (±10% of the experimental values).

The ZFSs of transition metal complexes have been previously believed to be strongly dominated by the spin-orbit coupling contribution that were frequently been interpreted by ligand field models. However, the conventional wisdom has recently been challenged and the latest theoretical results indicate that the spin-spin contribution is much larger than previously assumed [7]. Thus ligand field models often give very unrealistic results (or the fitted values have little relevance) since they almost never take account of the spin-spin interactions and rarely treat the important spin-flip contributions correctly. The quality of the linear response DFT method appears to be about the same as for the *g*-tensors and hence significant deviations from the experimental values are not uncommon.

However, the possibility to compute ZFSs from DFT is still a new development and much more experience is needed before conclusions can be drawn that are based on a sufficiently large body of experience.

What about environmental effects?

Even if the treatment of isolated molecules in the gas phase (the best case scenario) would be perfect, it would still be a substantial challenge for theory to correctly model many systems of interest for experimentalists. The challenges already start for the seemingly second best situation: molecules in inert gas matrices at low temperatures. For small radicals (e.g. CN, CO^+, BO) different experimental studies report *g*-shifts that differ by hundreds of ppm. Thus, accurate experimental data for such molecules that could be used for very high level calibration studies is lacking which is unfortunate for the further development of accurate theoretical approaches.

At the next level of sophistication radicals in solution require special attention since solvent shifts can be significant. Fortunately, even the crudest modeling of such effects by continuum dielectric approaches (such as PCM or COSMO) appears to be adequate as long as the solvent does not have specific directed interactions (such as hydrogen bonds) with the system of interest [44]. If there are hydrogen bonds, there is no substitute for explicitly including solvent molecules in the quantum chemical calculations. The combination of a few solvent molecules in conjunction with dielectric continuum methods has led to happy results in many cases. There is, however, still a substantial problem, since the potential energy surfaces for weakly bound solvent molecules must have many energetically close minima and any geometry optimization only finds the minima that are closest to the starting point. Thus, great care has to be exercised in such studies.

A more rigorous modeling of hydrogen bonds and related interactions is provided by first principle molecular dynamics approaches (Car-Parinello (CPMD) or Born-

Oppenheimer (BOD) dynamics). In such calculations one samples a sufficiently long trajectory of the molecule of interest in interaction with the solvent molecules. EPR properties are computed at a large number of 'snapshots' until they converge to well defined mean values [45, 46]. As an additional benefit, one obtains temperature effects and inhomogeneous contributions to the linewidth in such calculations. However, the effort for such studies is extremely high in terms of computer time and with respect to the large number of technical details that need to be taken care of. First-principles molecular dynamics approaches are hence still far from belonging to the standard arsenal of quantum chemistry.

Finally, in the case of proteins, the protein environment may exhibit significant effects on the EPR properties of active sites. While fairly large models of the active sites can nowadays be included in the modeling, a real protein consists of thousands of atoms and needs to be solvated by several tens of thousands of water molecules. The long range electrostatic effects of these additional atoms may end up changing the electronic structure of the active site significantly. Such systems are best treated by a combination of accurate quantum chemistry (for the active site) with cheap and crude molecular mechanics methods for the rest of the protein (QM/MM method). Very few studies have so far attempted to compute EPR properties of proteins on the basis of QM/MM methods [47] and many more are expected to follow. Again, both the computational and technical efforts for such studies are high.

Concluding remarks

This short exposition hopefully provides a reasonable feeling of what is possible with contemporary theory and what is not. It is fair to say that since the mid-nineties theory has come a long way to become an ever stronger partner of EPR spectroscopy. Density functional programs have almost matured and are readily available to the practicing EPR spectroscopist. Theory presently evolves in the direction of more challenging subjects such as the systems dynamics, excited states, infinite systems or relativistic effects. Yet, it is equally clear that further improvements in both the efficiency and the accuracy of the theory are highly desirable and appropriate approaches are being developed. The prospects for an accurate theoretical EPR spectroscopy appear to be bright.

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Validation of Distance Distributions Derived from DEER/PELDOR/DQ-EPR Data

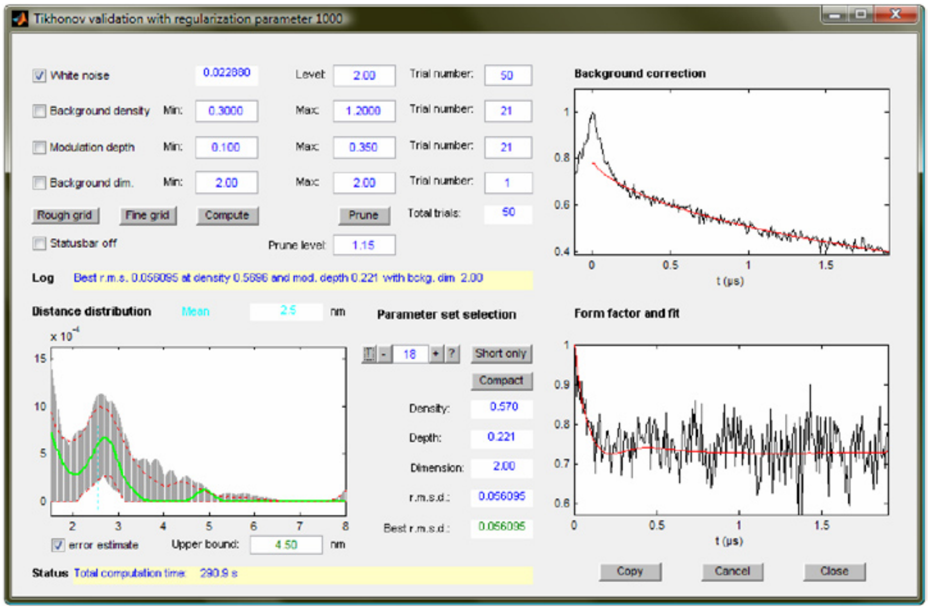
Gunnar Jeschke
ETH Zürich, Switzerland

The noise issue in distance measurements

Reliable and complete analysis of spectra requires a good signal-to-noise ratio (SNR). For a spectrum obtained in a field- or frequency sweep, noise can be estimated quite intuitively by looking at a printout. The same is true when the spectrum is obtained from time-domain data by a linear transformation. An example are ESEEM spectra that are obtained by Fourier transformation. In a linear transformation white noise in the primary data converts to white noise in the spectra and thus can easily be recognized. A different situation is encountered when a dipolar evolution function is transformed to a distance distribution. This transformation is non-linear and involves an ill-posed problem, where small changes in the input data can induce large changes in the output data. Ill-posed problems are solved by introducing additional constraints on the output data. In the case at hand, the distance distribution is required to be reasonably smooth and non-negative. These constraints can be implemented in several ways, for instance by Tikhonov regularization [1–3], or by the maximum entropy method [4]. Such mathematical trickery hides the influence of noise and of other distortions of the input data. Hence, a reasonably looking distance distribution may result from input data that are actually void of any information.

Clearly, this situation requires much caution in the interpretation of distance distributions. It is good practice to closely examine the input data of Tikhonov regularization, i.e., the form factor obtained by background correction of the primary measured data. The distance distribution is meaningless if the modulation depth does not significantly exceed the noise level or baseline rolling from incomplete background correction. The distance and the width of the distance distribution are reliable if several periods of a clear oscillation are observable in the form factor. If four or more periods are observable, even asymmetries in the shape of the distribution can be safely interpreted.

Some people maintain that only data with such clear oscillations should be used at all. However, molecular modeling and experience with spin-labeled protein samples show that, due to conformational distributions, the width of distance distributions is often so large that the oscillation is overdamped. If the modulation depth and the signal-to-noise ratio are sufficient, reliable interpretation of such data is still possible and structural models can be obtained [5, 6]. Thus the question arises: How reliable are broad distance distributions at a given signal-to-noise ratio and for given uncertainties in background correction?


Tikhonov validation with regularization parameter 1000

☑ White noise 0.022880 Level: 2.00 Trial number: 50
☐ Background density Min: 0.3000 Max: 1.2000 Trial number: 21
☐ Modulation depth Min: 0.100 Max: 0.350 Trial number: 21
☐ Background dim. Min: 2.00 Max: 2.00 Trial number: 1
Total trials: 50
☐ Statusbar off
Prune level: 1.15

Log Best r.m.s. 0.056095 at density 0.5696 and mod. depth 0.221 with bckg. dim 2.00

Distance distribution Mean 2.5 nm

Parameter set selection 18
Density: 0.570
Depth: 0.221
Dimension: 2.00
r.m.s.d.: 0.056095
Best r.m.s.d.: 0.056095

☑ error estimate
Upper bound: 4.50 nm

Status Total computation time: 290.9 s

A Monte Carlo approach to the validation of distance distributions

The reliability of the distance distribution can be estimated by error analysis. Given quantitative estimates of errors in the input data the error in the output data can be calculated according to the theory of errors. For an ill-posed problem such error analysis has to be performed numerically. In DeerAnalysis2008 [7, 8] this is done by creating many data sets within the input error bounds. These data sets are transformed to distance distributions by Tikhonov regularization so that an ensemble of distance distributions results. By statistical analysis of the ensemble error bars can be derived for each point $P(r)$ in the distance distribution.

This error analysis is initiated by the Validation button in DeerAnalysis2008. The button is clickable only after an initial Tikhonov regularization of the input data. This initial Tikhonov regularization provides an appropriate regularization parameter, for instance by using the L curve criterion [3], and an estimate for the SNR in the input data. The SNR is computed from the fit of the input data by the distance distribution obtained during initial Tikhonov regularization. The root mean square deviation (r.m.s.d.) of the form factor fit from the experimental form factor is interpreted as the root mean square amplitude of white noise. Note that the fit residual may have contributions that do not stem from white noise, but from inappropriate background correction. To see if this is the case, the fit residual should be examined, which is possible in DeerAnalysis2008 by selection of the Residual tickbox. If the residual is dominated by baseline rolling a different background model should be tried. Otherwise, both the distance distribution and its error estimate will be wrong.

▶

In many cases, background correction parameters are also somewhat uncertain. For instance, for membrane proteins reconstituted into liposomes the spatial distribution of spin labels in neighboring protein molecules is approximately two-dimensional, corresponding to background dimensionality $D \approx 2$. Experiments on singly labeled membrane proteins reveal that D varies somewhat between different labeling sites. Hence, for a doubly labeled protein only lower and upper bounds for D may be known. If the mean distance is long, background fitting is generally complicated. Reasonable background fits may then be obtained over a certain range of modulation depths and background densities.

The validation tool in DeerAnalysis2008 (see screenshot) allows to simultaneously test for several error sources. For noise tests, the noise level is increased by a constant factor (usually a factor of two). This is done by adding normally distributed pseudorandom numbers to the data. Background density k, modulation depth λ, and background dimensionality D are varied linearly within their bounds. For each analyzed parameter, a number of trials can be selected. The total number of trials is the product of all the single numbers. That way no correlation between parameters is assumed and all combinations are tested. If several background parameters are varied, the total number of trials may be rather large and computation time correspondingly long. It is then advisable to set the number of noise trials to 1. This is permitted as different white noise with the preselected noise level is added in each of the trials, even if only background parameters are varied explicitly.

The ensemble of distance distributions from all trials is analyzed by computing for each point $P(r)$ the mean value $\langle P \rangle$ and standard deviation σ_P. Grey error bars in the distance distribution display indicate the minimum and maximum value of $P(r)$ throughout the whole ensemble, while the red dashed lines are bounds corresponding to $\langle P \rangle \pm 2\sigma_P$.

The data in the screenshot correspond to double mutant 328/346 of the sodium/proline symporter PutP [6]. Error analysis reveals that only the peak between 2 and 3 nm is highly significant. Both the feature at distances shorter than 2 nm and the feature at about 5 nm are within the noise level. A distance between 2 and 3 nm is indeed in agreement with the α-helical structure of this part of the peptide chain. Note however that the error estimate corresponds to twice the noise level of the original data. This doubling may lead to an overestimate of the error. In a situation like this, with poor SNR, it is advisable to repeat error analysis with a noise level factor of only 1.5. For PutP double mutant 328/346 such a test still indicates that the features at very short and very long distances are noise related (data not shown).

Limitations

In fact, background parameters are correlated, i.e., not all combinations of parameters result in an appropriate background correction, even if each single parameter is chosen between its lower and upper bound. The bad parameter combinations may lead to a strong overestimate of the errors in the distance distribution. Such bad combinations of background parameters can be recognized, as they correspond to poor fits of the form factor. Thus the r.m.s.d. between this fit and the experimental form factor is significantly larger than for good parameter combinations. The ensemble can be pruned to reasonable parameter combinations by rejecting all distance distributions that correspond to poor fits. In DeerAnalysis2008 this is done by clicking on the Prune button after the computation. By default an r.m.s.d. larger than 1.15 of the minimum r.m.s.d. of all data sets is considered as a poor fit. If necessary, the prune level can be adjusted by the user.

Final remark

DeerAnalysis2008 was updated on January 6th 2009. The description above corresponds to the updated version. Suggestions for improvement and comments on performance are always welcome and should be directed to gunnar.jeschke@phys.chem.ethz.ch.

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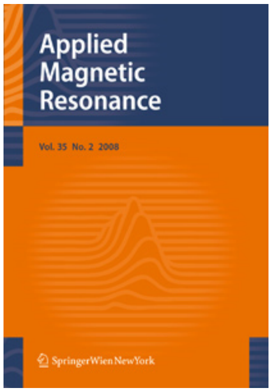

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High-Field EPR Spectroscopy on Proteins and Their Model Systems

by
Klaus Möbius and
Anton Savitsky

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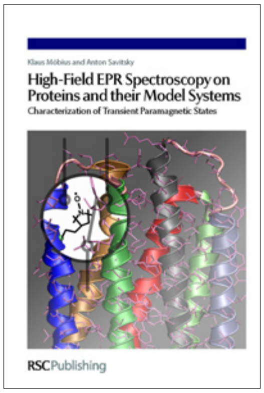
BIC: PNFL, PSBC



Synopsis
The book offers a comprehensive overview of experimental techniques in, and paradigmatic examples of, the application of high-field EPR spectroscopy in biology and chemistry. The authors focus on the use of the technique in conjunction with site-specific mutation strategies and advanced quantum chemical computation methods in order to reveal protein structures and dynamics. Theory, practice and future perspectives are covered. This book is an indispensable resource of essential reading for scientists, academics and postgraduate students.

Brief Contents
Introduction
Principles and illustrative examples of high-field/high-frequency EPR spectroscopy
Instrumentation
Computational methods for data interpretation
Applications of high-field EPR on selected proteins and their model systems
Conclusions and perspectives

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Reader's Corner

Keeping the Flame Burning – Using Magnetic Resonance To Keep Kids Interested in Science (Part Three)

by Reef Morse
Steppingstone Magnetic Resonance Training (SMART) Center
reef@smart-center.org
www.smart-center.org

There are now two presentations available on the web site – one for imaging, and one for resonance as described in the previous column. These are available for anyone under the GNU Copyleft – that is, please acknowledge the source of these materials when you use them.

One of the important functions of the SMART Center is to act as a model for ways that scientists, young and old, can communicate their passion about science to the nonscientific community. Educating the larger public about what we do and how we do it is an important aspect of our craft. Most of us depend on public funds to do our work but few people outside the funding agencies have any idea what we do. If you want a good demonstration of this, go into a bar, sidle up to someone, and say you are a physical biochemist. Most people will respond as if you were a rabid animal.

Few people educated in the US will have had classes in science much beyond high school (12th grade) and most of them will have had only one or two science classes beyond 8th grade. Teachers teaching Science at the elementary school level have degrees in elementary education, not science. In the US, elementary school teachers are not required to have an additional major. They can, for the most part, teach out of a book, but cannot communicate the real details of science that makes it so fascinating for scientists.

I'd be interested in comments regarding the above observation(s) and in learning more about what you, my colleagues, are doing in the way of public interaction. What is the general response to people in other countries to "science" and "scientists"? Please reply through the email address above.

Hopefully, by the time this article is in your hands, the ESP300 donated by Bruker BioSpin should be up and running. We've been waiting for a magnet and power supply and a delivery date. The plan is to introduce the SMART Center instrumentation to local public school officials. Next will be an extensive outreach program to science clubs and science teachers in our area. Our target date for opening the center for instrument training is April to May, and we should begin working on an imaging project by the summer.

Notices of Meetings

The 42nd Annual International Meeting of the Electron Spin Resonance Group of the Royal Society of Chemistry

Norwich, United Kingdom, April 19–23, 2009
www.uea-epr.eu

Gordon Research Conferences. Magnetic Resonance

University of New England Biddeford,
Maine, USA, June 14–19, 2009
www.grc.org

EUROMAR Congress 2009

Göteborg, Sweden, July 5–10, 2009
www.euromar2009.com

The 11th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena

Brock University, St. Catharines, Ontario,
Canada, August 9–14, 2009
www.brocku.ca/scm09

7th European Federation of EPR Groups Meeting and Closing Meeting of COST P15

Antwerp, Belgium, September 6–11, 2009
www.efepr2009.ua.ac.be

The 10th International Conference on Magnetic Resonance Microscopy (ICMRM 10)

West Yellowstone, Montana, USA
August 30 – September 3, 2009
www.icmrm10.montana.edu

International Workshop Electron Magnetic Resonance of Strongly Correlated Spin Systems (EMRSCS2009)

Kobe, Japan, November 8–9, 2009
extreme.phys.sci.kobe-u.ac.jp/EMRSCS2009

Molecular Photoscience Research Center, Kobe University will be organizing an international workshop "Electron Magnetic Resonance of Strongly Correlated Spin Systems" on November 8 and 9, 2009, prior to the 48th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2009) in Kobe. This international workshop will cover the recent advances of high frequency and high field EMR and its applications to the study of strongly correlated spin systems. Invited speakers from overseas include O. Cepas (France), S. Demishev (Russia), O. Portugall (France), G. Smith (UK), J. van Tol (USA), S. Zvyagin (Germany). The deadline for the submission of the abstract is August 10, 2009. For further information, please see the web site or contact:

Hitoshi Ohta (Chairperson), Eiji Ohmichi (Secretary), Organizing Committee, e-mail: emrscs@ruby.kobe-u.ac.jp

The 48th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2009)

Kobe, Japan, November 10–12, 2009
extreme.phys.sci.kobe-u.ac.jp/sest2009

SEST2009 will be held at the Centennial Hall of Kobe University during November 10-12. This is the 48th Annual Meeting of the Society of Electron Spin Science and Technology. The conference site, where the APES2001 was held previously, gives a splendid view of the sea, and the annual meeting will cover the wide range of EPR/ESR applications in physics, chemistry, biology and medicine. Following the tradition of the annual meeting of SEST, several distinguished scientists from overseas, including G. Smith (UK), will give plenary lectures at the meeting. Participants from all over the world are welcome. For further information, please see the web site or contact:

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The University of New Hampshire invites

The Department of Chemistry at the University of New Hampshire welcomes inquiries from PhD scientists at any rank regarding research, and graduate and undergraduate teaching opportunities, in the area of Experimental Physical or Biophysical Chemistry. Candidates with research interests in electron resonance are particularly encouraged. Facilities include Bruker ELEXSYS E500/E560 with X-band CW-ENDOR, and Varian X- and Q-band CW-EPR/ENDOR spectrometers with dispersion and absorption mode detection and temperature capability from 2 to 300 K. The electron resonance lab has a variety of microwave components, bridges, cavities and electronic measuring equipment for instrument construction as well as facilities for biochemical research. Inquiries should include a cover letter explaining the type of research and teaching opportunities desired, a CV, research plans and teaching goals, and should identify three people as references. Send to: Christopher F. Bauer, Chair, Department of Chemistry, University of New Hampshire, Durham, NH 03824 (603) 862-1550 (fax 4278), cfb@cisunix.unh.edu. Inquiries will be reviewed as they are received. UNH supports diversity and strongly encourages women and minority candidates to send an inquiry.

Research Positions - Advanced EPR of Bioinorganic Systems

Several research positions (PhD and Postdoc level) are presently available in the EPR department of the Max Planck Institute of Bioinorganic Chemistry in Mülheim/Ruhr, Germany.

We are looking for highly motivated young scientists in the field of Electron Paramagnetic Resonance who are interested in studying metallo-enzymes and related model systems. The main focus is on the investigation of photosynthetic systems (reaction centers, water oxidation), hydrogenase (biohydrogen production), radical enzymes and protein maquettes.

Our EPR lab is equipped with the full range of modern Bruker EPR spectrometers including E500 CW X-band, E580 CW/pulse X-band, E700 CW/pulse Q-band, and E680 CW/pulse W-band. In addition a high field CW/pulse spectrometer operating at 122 and 244 GHz (fields up to 12 T) is available next to several other CW EPR systems at S-, C-, X- and Q-band. We are using the complete repertoire of pulse and CW EPR techniques (ENDOR/TRIPLE, ELDOR, ESEEM) in combination with laser excitation and freeze quench techniques. More details can be found on our website: www.mpibac.mpg.de/lubitz.html.

The selected persons should have relevant training in Magnetic Resonance Spectroscopy, preferably in EPR. Candidates with an interest in EPR instrumental development and microwave engineering are specifically encouraged to respond.

Please send your application to Prof. Dr. Wolfgang Lubitz, Max Planck-Institute for Bioinorganic Chemistry, Stiftstrasse 34-36, 45470 Mülheim an der Ruhr, Germany

E-mail: lubitz@mpi-muelheim.mpg.de

Postdoctoral or Research Associate position

A position on pulse EPR at the postdoctoral or research associate level depending on qualifications is available at the CNR-INFM MDM National Laboratory, in Agrate Brianza (Milano, Italy). The research activity is related to the pulse EPR/ENDOR investigation of impurities in semiconductors for quantum information processing. The successful candidate must have experience on the pulse EPR/ENDOR techniques possibly connected with the study of semiconductors or insulators, excellent knowledge of solid state physics and quantum mechanics, and good experimental skills. The position is initially for one year, but can be renewed up to five years. For additional information **please contact:** Prof. Marco Fanciulli, marco.fanciulli@mdm.infm.it, tel. +390396036253 (direct), +390396037489 (secretary).

Postdoctoral position at Physics Department, National Dong Hwa University, Taiwan

A postdoctoral position is available in the laboratory of Prof. Shyue-Chu Ke at the Physics Department, National Dong Hwa University, Taiwan. The research will involve the application of EPR and pulsed EPR spectroscopy to understand the fundamental questions related to adenosylcobalamin-de-

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pendent enzymatic reactions. Additional information about the laboratory is available at: www.phys.ndhu.edu.tw/teachers/ke/ke.htm. Applicants should have experience in analytical techniques and continuous or pulsed EPR methods and data analysis. Experimental physical chemists with experience in cell culture or synthesis would be beneficial, but is not essential. The position is available this summer and appointments are for up to 3 years. If interested, please send a CV and summary of previous research experience to ke@mail.ndhu.edu.tw.

Tenure-Track Faculty position in Physical Chemistry

The Department of Chemistry at the University of New Hampshire invites applications for a tenure-track faculty position at the rank of assistant professor in any area of Experimental Physical Chemistry. The Department has extensive electron resonance facilities and is active in atmospheric science and nanotechnology. Candidates with expertise in these areas may enjoy significant opportunities for collaboration. The Departmental mission balances research and teaching: A commitment to high quality undergraduate and graduate education, and to establishing a vigorous, nationally-recognized research program, are essential. PhD required. Interested candidates should send curriculum vitae, undergraduate and graduate transcripts, research plans, evidence of teaching proficiency and philosophy, and three letters of recommendation to Christopher F. Bauer, Chair, Department of Chemistry, University of New Hampshire, Durham, NH 03824 (603) 862-1550 (FAX 4278), cfb@cisunix.unh.edu. Review of applications will commence on November 20, 2008. UNH supports diversity among its faculty and strongly encourages women and minority candidates to apply.

EQUIPMENT

Design and construction of ESR modules

The Magnetic Resonance laboratory at the Israel Institute of Technology has developed a variety of electronic modules, systems and probes for ESR and NMR. We are open to disseminate these projects and share our designs and modules either in a collaborative or in a service mode of action. Major recent instrumentation projects include: (1) 6–18 GHz pulsed ESR microwave bridge; (2) 33–36 GHz pulsed ESR microwave bridge; (3) 6–18 GHz CW ESR microwave bridge; (4) Pulsed gradient drivers for ESR and NMR (for imaging and/or field jump experiments); (5) Retrofitted Lakeshore Magnetic Field controller with improved resolution; (6) Retrofitted Walker electro-magnet power supply with improved stability.

Contact details: Aharon Blank,
ab359@tx.technion.ac.il
Web address: www2.technion.ac.il/~ab359

Available: EPR accessories and supplies

We have some excess EPR accessories and supplies that might be of use to other labs. For example, we have a lot of chart paper, pens and ink for older recorders, and some spare parts and accessories such as VT Dewars for older spectrometers. If you need something for an older-style Varian or Bruker spectrometer, ask us – we might be able to help. Most items are available for shipping costs.

Gareth R. Eaton geaton@du.edu

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-, L-band, or MHz 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.

Please contact: Richard W. Quine, e-mail: rquine@du.edu, phone: 1-303-871-2419

For sale: Varian and ESR equipment

Resonance Instruments has available: (1) Replacement klystrons for Varian EPR bridges and some Bruker bridges (at reduced prices) and other klystrons; (2) Resonance Instrument's Model 8320A is a general purpose Hall-effect based magnetic field controller that provides direct control and precise regulation of the magnetic field between the pole pieces of an electromatnet. Its high resolution permits precise adjustment of the magnet's field either though the front panel keyboard or though an RS232 serial interface with your PC.

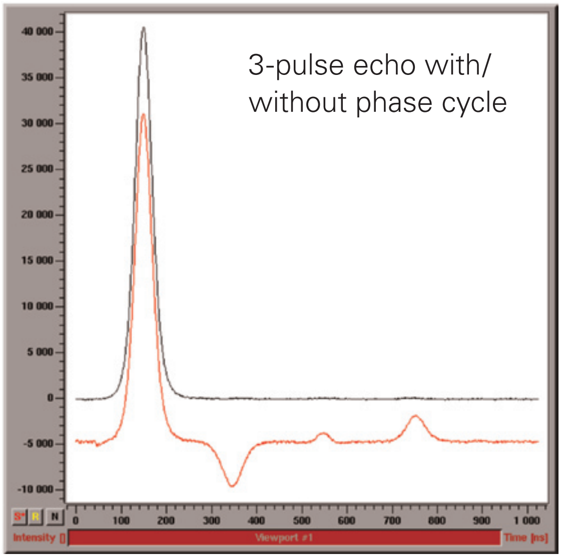
Please contact:
Clarence Arnow, President, e-mail: 8400sales@resonanceinstruments.com, phone: 1-847-583-1000, fax: 1-847-583-1021.

Available: Used Varian EPR equipment

(1) Varian E-104 EPR spectrometer with vertical style bridge and e-line fieldial. (2) Varian E-9 EPR spectrometer. Both available with warranty and continued service support. (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.

Please contact: James Anderson, Research Specialties, 1030 S. Main St., Cedar Grove, WI 53013, USA.
phone/fax: 1-920-668-9905
e-mail: janderson36@wi.rr.com

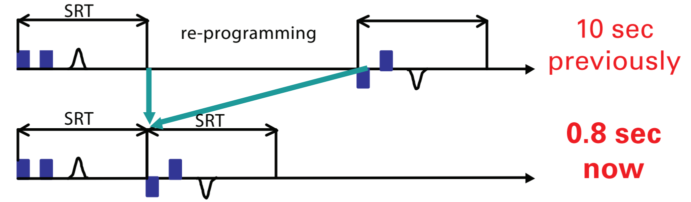
Bruker BioSpin



PatternJet-II timing

Reducing re-programming overhead by high speed Direct Phase Cycling (DPC)

Measuring time for 2 pulse echo with 16 step phase cycle



E 580 Evolution

Combining the unique features of SpecJet-II and PatternJet-II, it is now possible to perform high speed phase cycling without reprogramming overhead. For example, the full time evolution, including all phase cycles of an ESEEM experiment, is preloaded into the PatternJet-II memory and executed without any interrupts.

Leading performance from the company synonymous with EPR www.bruker-biospin.com

think forward

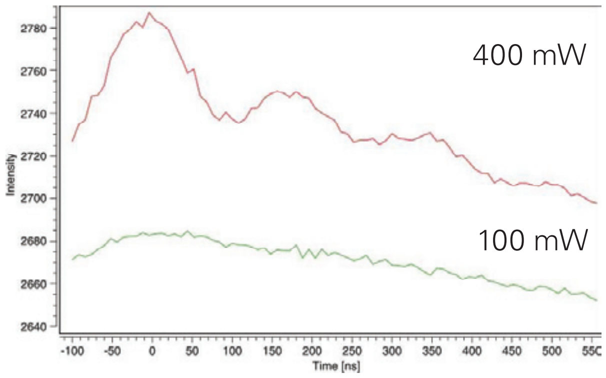
EPR

W-Band EPR 6T SC

- **2000 G high resolution sweep coil**
- **Automatic sweep linearization**

W-Band high power

- **400 mW pulse power**



New pulse power module with 400 mW

- 16 ns $\pi/2$ pulse
- Improved DEER modulation

E 680 Evolution

The E 680 W-Band spectrometer has evolved to the next performance level. The new 6T magnet surpasses all previous designs in specifications and ease of handling.
The new power module for pulse EPR pushes the power level up to 400 mW, reducing $\pi/2$ pulses to 16 ns thereby greatly enhancing the performance of DEER measurements.

Leading performance from the company synonymous with EPR www.bruker-biospin.com