Spectroscopy Society of Pittsburgh January Meeting

Duquesne University – Mellon Hall of Science (Laura Falk Hall)

Wednesday – February 10, 2010

Technology Forum Speaker's Presentation **5:30PM**
Social Hour **6:00PM**
Dinner in the City View Café (6th Floor) **6:30PM**
Business Meeting **8:00PM**
Technical Program Speaker's Presentation **8:15PM**

Deadline for Dinner Reservations **2/5/10**
Carolyn Benga crbssp@yahoo.com or (412) 487-0915

TECHNOLOGY FORUM - 5:30 PM
Dr. John E. Rawlins, Carnegie Museum of Natural History

"Bug Therapy: Discovering How Insects Make Our World Better"
In diverse ways, insects and related arthropods are increasingly playing an important role in improving the quality of life for human beings. Innovating new ways to use old bugs is part of the mission of curators in the Section of Invertebrate Zoology at Carnegie Museum of Natural History. In this short talk Dr. Rawlins provides a glimpse into the daily life and challenges of a curator in a world-class insect collection, clarifies how the resource of specimens, data, and staff expertise are harnessed to address traditional challenges, and through technological innovation, to answer new questions and needs for our future. Rawlins discusses his involvement with bugs aided by current technology: scanning electron microscopy, auto-montage imaging, x-ray analytical methods, and forensics and identification procedures, as well as aspirations for future notions (bugs-to-drugs, entomological inspiration for robot development, and more).

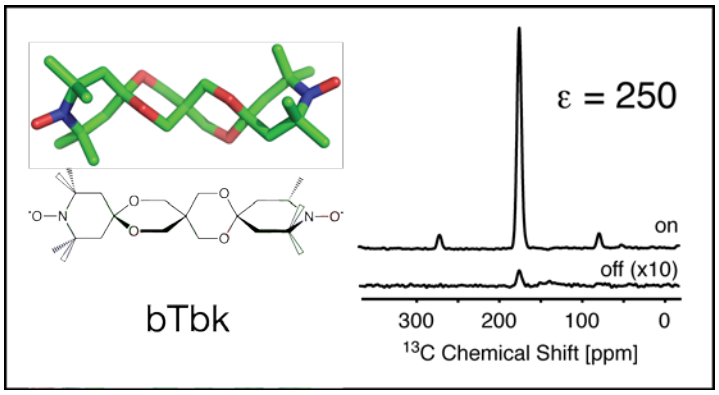
Bio
Rawlins grew up on a sheep ranch in eastern Oregon, received a Bachelor of Science degree from Oregon State University in vertebrate zoology and a doctorate from Cornell University in systematic entomology, worked as an Assistant Professor of Zoology at University of Texas, Austin, and for the last 25 years as been at Carnegie Museum of Natural History as the curator in charge of the Section of Invertebrate Zoology. Research interests emphasize natural history and phylogeny of Lepidoptera with special emphasis on the immature stages of moths, biotic inventory involving insects, and use of insects as indicator systems for environmental change, conservation, and resource management. He is interested in topics integrating technology with insects and their kin (e.g., using arthropod structure and function as biomodels in robotics). Current projects include NSF-sponsored biotic inventory of invertebrates and plants on Hispaniola, NSF-sponsored inventory of butterflies in Ghana, molecular and morphological studies on phylogeny of world cutworm moths and their relatives, federally funded State Wildlife Project for Invertebrate Species of Special Concern in Pennsylvania, and collaborative work on Neotropical ghost moths and Pennsylvania fireflies.

TECHNICAL PROGRAM - 8:15PM
R. G. Griffin, Francis Bitter Magnet Laboratory and Department of Chemistry Massachusetts Institute of Technology

"Dynamic Nuclear Polarization Nuclear Magnetic Resonance in Liquids and Solids at High Magnetic Fields Why Two Electrons Are Better Than One"
Nuclear magnetic resonance (NMR) is probably the most versatile analytical technique available to chemistry and biochemistry because it is non-perturbing and offers site-specific atomic resolution available with few other approaches. It is very forgiving as to the physical state of the sample, being applicable to gases, solutions and to amorphous and crystalline and microcrystalline solids. In addition, for similar reasons NMR (or MRI) is widely used in many other areas of science ranging from basic nuclear physics to medical imaging.

Despite its enormous versatility, the sensitivity of the NMR experiments is relatively low because it is based on observation of low energy spectroscopic transitions between nuclear Zeeman levels. As a consequence, there are continuing efforts to develop new NMR methods and instrumentation that improve the signal-to-noise of the experiments. Some of the most successful of these involve polarization transfer experiments that move polarization from a highly polarized spin reservoir to a weakly polarized one, leading to an enhancement in the NMR signal intensities proportional to the ratio of the magnetic moments of the two spin species. It is now appreciated that the largest gains in signal intensities in these sorts of experiments can be achieved by transferring polarization from an electron spin(s) to a nuclear spin system. This is generally accomplished via microwave irradiation of the electron paramagnetic resonance (EPR) spectrum, an experiment known as dynamic nuclear polarization (DNP) NMR. Since contemporary NMR experiments are performed at magnetic fields of ~5-23 T, the required microwave radiation falls into the frequency range 140-660 GHz, or the millimeter wave regime. This presentation discusses the implementation of DNP/NMR experiments in high magnetic fields.

Over the last few years we have developed cyclotron resonance maser (a.k.a. gyrotron) microwave sources that operate at frequencies of 140-460 GHz that permit DNP enhanced NMR (DNP/NMR) experiments in magnetic fields of 5-16.4 T (1H NMR frequencies of 211-700 MHz, respectively). We review the instrumentation used for these experiments, which include new NMR probe designs and tunable gyrotron sources. In addition, we discuss two mechanisms that are currently used for DNP experiments in solids at high fields – the solid effect and cross effect -- and the polarizing agents appropriate for each. These include biradicals that enable increased enhancements at reduced concentrations of the paramagnetic center. Figure 1 depicts recent results obtained from the rigid biradical bis-TEMPO-bis-ketal (bTbk) where we observe an enhancement of ~250, or a reduction in signal averaging time of 62,500. In addition, we discuss applications of DNP/NMR that illustrate its utility in enhancing signal-to-noise in MAS NMR spectra of a variety of biological systems including membrane and amyloid proteins whose structures are of considerable scientific interest. Presently, enhancements that are routinely available and range from 40-250 depending on experimental variables such as temperature, magnetic field, microwave B1, polarizing agent, etc. Finally, we describe extensions of these experiments that permit observation of 13C liquid state spectra where we have observed enhancements of 140-400 in small molecules and a protein..



Bio

Prof. Robert G. Griffin received his B.S. degree (with Honors) in 1964 majoring in Chemistry at the University of Arkansas. He attended graduate school at Washington University (St. Louis, MO) where he worked with Prof. Samuel I. Weissman on EPR experiments directed at understanding the spectra and electron transfer processes of radical ions in solution. In 1970 after completing his Ph.D., he moved to MIT to perform postdoctoral work with Prof. John S. Waugh. At that time the field of high resolution NMR in solids was in its infancy, and he was involved in multiple pulse NMR experiments that reported the initial observation of chemical shift anisotropies in single crystals and powders. In 1972 Prof. Griffin accepted a position at the Francis Bitter Magnet Laboratory (FBML) as a staff scientist, and rose through the ranks to become Director in 1992. He joined the faculty of the MIT Chemistry Dept. in 1988 where he teaches physical chemistry. In 2007 Professor Griffin received the Eastern Analytical Symposium Award for Outstanding Contributions to Magnetic Resonance and the Günther Laukien Prize of the Experimental Nuclear Magnetic Resonance Conference. In 2008 he was elected a Fellow of the International Society of Magnetic Resonance (ISMAR), and an honorary fellow of the NMR Society of India in 2009. In 2010 he received the ISMAR Prize for the development of high frequency dynamic nuclear polarization experiments.

Dinner Reservations:

Please email Carolyn Benga at crbssp@yahoo.com or call (412) 487-0915 to make dinner reservations NO LATER THAN FRIDAY, February 5, 2010. This month's dinner is a celebration of Xin Nian Kuai Le, Chinese New Year. The entrée will be Shrimp with Broccoli in Brown Sauce served over White Rice. Vegetable Egg Rolls will begin the meal and Lemon Pound Cake will be served for dessert along with Fortune Cookies. Dinner will cost

$8 and checks can be made out to the SSP. If you have dietary restrictions, please let Carolyn know when you RSVP.

Parking Instructions:
The Duquesne University Parking Garage is located on Forbes Avenue. Upon entering the garage, receive parking ticket and drive to upper floors. Pick up a parking chit at the dinner or meeting. If any difficulties arise, contact Dr. Mitch Johnson at Duquesne University.