

# CINTACS



Newsletter of the Cincinnati Section of the American Chemical Society February, 2003  
Vol. 40, No. 6

## Calendar

### *New online registration!*

Wednesday, February 12	Dr. Paul Lahti at Vernon Manor
Wednesday, March 12	Cincinnati Chemist at Givaudan
Wednesday, April 9	Mr. Frederick Wallace at Northern Kentucky
Friday, May 16	Party Night! Robert Mondavi Montgomery Inn Boathouse

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## *Design of Molecular Magnetic Materials*

**Paul M. Lahti**

Department of Chemistry, University of Massachusetts, Amherst

### Abstract

The stable radical 5-(4-[*N-tert*-Butyl-*N*-aminoxyl]phenyl)pyrimidine (PyrimPhNIT) forms both 1:1 and 2:1 complexes with  $M(\text{hfac})_2$ , ( $M=\text{Mn, Co, Ni, Cu, Zn}$ ). The 2:1 complexes are isostructural, as shown below. Magnetically, they exhibit mostly spin pairing between adjacent radical spin units, and little interaction with the metal cations. The 1:1 complexes are cyclic systems showing strong antiferromagnetic (AFM) ( $M=\text{Mn}$ ) or FM ( $M=\text{Cu}$ ) exchange between metal and nitroxide units. There is AFM intramolecular exchange between M-NIT sites in both complexes, as we have previously noted (Field, L. M.; Lahti, P. M.; Palacio, F. *Chem. Comm.* **2002**, (6), 636-637). Although the AFM intersite exchange can be attributed to *intramolecular* spin polarization effects, there is also an excellent *intermolecular* orbital-overlap arrangement between pyrimidine

*(Continued on page 4)*

### About the Speaker

Paul M. Lahti was born and raised in Massachusetts. He did his undergraduate work at Cornell University (A.B. 1978 with Distinction; George Caldwell Prize in Undergraduate Chemistry 1978), and his M.S. (1980), M.Phil. (1981) and Ph.D. (1985) degrees at Yale University under the guidance of Jerome A. Berson in the area of physical organic chemistry of open-shell molecules. He was a National Science Foundation Pre-doctoral Fellow during 1978-1981. He began his career as an educator as an Assistant Lecturer of Physical Chemistry at the University of the West Indies, Kingston Jamaica (1981-1983), and after completing his doctorate joined the chemistry department at University of Massa-

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**THE CINTACS NEWSLETTER****Vol. 40, No. 6 February, 2003**

Editor.....Bruce S. Ault  
 Advertising.....Ed Hunter

CINTACS is published nine times a year (September through May) by the Cincinnati Section of the American Chemical Society. The submission deadline will be approximately February 19 for the April, 2003 issue. Electronic submission is strongly preferred, except for original photos. All materials should be sent to:

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**from the Chair**

The February meeting will be held at the Vernon Manor Hotel at 400 Oak Street in Clifton. (For you trivia buffs, this was the address given for the K-Mart in the movie *Rainman*.) The meeting is being generously sponsored by Rick Fayter, whom I would like to thank very much. As I mentioned in my last statement, without the meeting sponsors, it would be very difficult to hold our monthly meetings. The after-dinner speaker will be Prof. Paul Lahti from the University of Massachusetts in Amherst.

The anonymous donation we received last year specifically earmarked 25% of the interest for Project Seed. Unfortunately, this program has been inactive in the Cincinnati Section for a large number of years. Thus, we had to start from scratch, and as I said in my last statement, we needed someone to be the coordinator. I am happy to report that Joel Shulman, our Chair-elect, has taken it upon himself to be the coordinator for Project Seed. He has found three faculty members at UC who are willing and eager to take high school students into their laboratories for the summer. Joel and Linda Ford are contacting local schools to find the appropriate students.

The funding for Project Seed comes from a number of sources. As mentioned above, some money comes from the anonymous donation. In addition, at the last meeting, the Board agreed to make a donation from its general funds. Each of the three faculty members will contribute to the salaries of the students and will cover all of the laboratory expenses. Finally, Joel is writing a grant proposal to ACS National to cover about half the students' salaries. Thus, because of Joel, we are off to a great start.

If you would like to donate to Project Seed, if you are a faculty member and would like a Project Seed student in your labs, if you are a high school teacher and know a good student for the program, or if you would just like to help, please contact Joel Shulman.

The March meeting will be the Cincinnati Chemist of the Year and the Cincinnati Research Associate of the Year Award presentations. In addition, Linda Ford will receive special recognition for her National ACS Teaching Award. The meeting will be held at Givaudan.

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**Central Regional Meeting**

This year, the Central Regional Meeting will be held in the Fall, October 19 - 22, at the Sheraton Station Square in Pittsburgh, PA. All members in the Central Region are encouraged to consider attending and participating in the many different activities that are planned.

**February Monthly Meeting  
February 12, 2003  
Vernon Manor Hotel  
400 Oak Street, Cincinnati**

*sponsored by Dr. Rick Fayer*

**Featured Speaker  
Professor Paul Lahti  
University of Massachusetts**

**Program**

6:00—7:00 pm registration, social hour and vegetable tray

6:00—7:00 p.m. Biochemistry Discussion Group  
Professor Richard A. Gibbs  
*"Chemical Probes of Protein Prenylation"*

7:00—8:00 p.m. buffet dinner (\$24 includes one drink ticket) Menu: salad, lemon chicken breast, roast top sirloin, red skin potatoes, dessert, coffee, hot and iced tea

8:00 pm meeting and featured speaker  
Professor Paul Lahti  
*Design of Molecular Magnetic Materials*

**Reservations:** New! A meeting reservation form is now online at: <http://www.che.uc.edu/acs/cinacs.html>. This is the best and easiest way to register. As a lesser alternative, you may send your reservations by email to [Kim.Carey@uc.edu](mailto:Kim.Carey@uc.edu). If absolutely impossible to make reservations via the internet, telephone 513-556-0293. Deadline for reservations is 12:00 noon on Friday, February 7, 2003. Include your name, affiliation, and state if you're in one of the 1/2 price categories. As a reminder, if you decide you must miss a meeting after you have made reservations, please call to cancel. If you do not cancel, the Section will have to charge you because it will have been charged by the hotel

**Directions:**

**From I-75:** Take the Hopple Street exit and at the light, take a left. Continue straight on Marin Luther King Drive past UC and past University Hospital. At Burnet Avenue, take a right. Continue on Burnet to Oak Street. The Vernon Manor hotel is on the left hand corner of Oak and Burnet with the front door on Oak.

**From I-71S:** Take the Taft Street exit. At the light at the end of the exit go straight. Take a right on Burnet, and continue on Burnet to Oak Street. The Vernon Manor hotel is on the right hand corner of Oak and Burnet with the front door on Oak..

*(Continued from page 1)*

units of different molecules of the Cu(II) complex. This latter situation exemplifies the possible dangers of using molecular connectivity as the major criterion for modeling or understanding exchange or magnetic behavior in the solid state.

Interestingly, PyrimPhNIT forms a 2:3 complex with Co(hfac)<sub>2</sub>, which shows a ribbon motif in the X-ray crystallographic analysis. This extended system involves coordination of all available sites in PyrimPhNIT, the only example that we have found so far where this is true. Comparisons to related organic molecules with similar extended crystallographic and magnetic ordering will also be made.

This work was supported by the National Science Foundation (CHE 0109094, CHE-9809548, CTS-0116498, CHE-9974648), the Comision Interministerial de Ciencia y Tecnologia of Spain (CICYT-MAT2000-1388-C03-03), and the Full-bright España commission.

*(Continued from page 1)*

achusetts at Amherst, where he has been on the faculty since 1985. He became full Professor in 1995, and an adjunct Professor in the Department of Polymer Science and Engineering in 2000. He has served both as associate head (1999) and head (1999-2002) in the chemistry department, has been awarded a College Outstanding Teaching Award (UMass-Amherst, 1994), and has developed many of the chemistry safety policies at his university. He is internationally recognized for his work in the area of molecular magnetism with organic molecules and materials, including a major book published with Marcel Dekker in 1999. He has also published three invited book chapters on various aspects of polymer chemistry. He has presented numerous lectures internationally, thanks to the kindness of superb collaborators. His main areas of scientific interest are electronic properties of molecules, polymers, and molecular solids; computer-interactive chemistry educational methods; spectroscopy of reactive intermediates.

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## Biochemistry Discussion Group

### "Chemical Probes of Protein Prenylation"

Professor Richard A. Gibbs  
Purdue University

Protein farnesyltransferase (FTase) transfers the farnesyl group from farnesyl diphosphate (FPP) to the cysteine sulfhydryl group in peptides and proteins having the carboxyl-terminal sequence CaaX, where X = methionine, serine, glutamine, or threonine. FTase is emerging as a key potential anti-cancer drug target, with three FTase inhibitors in current clinical trials. However, much remains to be learned about the biological consequences of FTase inhibition. Crystallographic studies on FTase have revealed that the farnesyl moiety forms part of the binding site on FTase for the peptide substrate. In accord with this structural insight, recent data in our laboratory has demonstrated that changing the structure of the isoprenoid side chain of FPP can alter the peptide substrate specificity of FTase. In particular, two FPP analogues that are alternative substrates for FTase with the prototypical CaaX box CVLS are inhibitors of the prenylation of peptides bearing the CaaX box CKVL. Based on this finding, we hypothesize that certain FPP analogs may inhibit the prenylation of a subset of proteins inside a cell, but still prenylate other protein targets.

Richard A. Gibbs is an Associate Professor of Medicinal Chemistry and Molecular Pharmacology at Purdue University. Professor Gibbs received his undergraduate education (B.A. in Natural Sciences, 1983) from Johns Hopkins University and his graduate education (Ph.D. in Organic Chemistry, 1988) from the University of California-Riverside. After serving as a Postdoctoral Fellow in the Department of Chemistry at Penn State University from 1988 through 1991, Dr. Gibbs started his academic career as an Assistant Professor in the Department of Pharmaceutical Sciences at Wayne State University in 1992. He was promoted to Associate Professor in 1998, and assumed his current position at Purdue in 2001. Dr. Gibbs has been

*(Continued on page 5)*

## Chemical Educators' Discussion Group

### Two Upcoming Events!

1. On Monday, February 24<sup>th</sup>, join us for "The History of the Chemistry Set". Bill Jensen, chemistry historian at the University of Cincinnati, has invited us to his chemistry museum to enjoy a very visual lecture on the evolution of the chemistry set from 1770 to 1980 and to view the extensive collection. For some of us who were enjoying our own chemistry sets in the 50's and 60's, it will be a trip down memory lane. For younger teachers it might very well be a I-can't-believe-they-let-kids-have-that experience. We will meet in the conference room (Room 518) of Rieveschl Hall at 6:30 PM for light refreshments and announcements. At 7 PM we will walk the short distance down the hall to Room 520 for the program. Please bring a friend or colleague for this special occasion.

**Directions:** You are heading for the main campus of the University of Cincinnati. From I-75, take the Hopple Street exit, turn left, and proceed up the hill toward campus. Hopple St. will turn into Martin Luther King Drive. When you get to the top of the hill, turn right onto Clifton Avenue and then make a quick left onto College Court. (College Court is nestled between the DAAP building and Wilson Auditorium.) This short drive will take you straight into a parking garage under Rieveschl Hall. **Park and bring your parking ticket upstairs with you. It will be validated with a stamp to save you the cost of parking.** From I-71, take the Taft Road exit and travel west toward campus. As you cross Vine Street, Taft Road becomes Calhoun Street. Stay on Calhoun until it dead ends into Clifton Avenue. Turn right onto Clifton Avenue and travel a short distance past several university buildings until you get to College Court. Turn right and travel back to the parking garage.

2. On Monday, March 3<sup>rd</sup>, join us for a meeting on "Instrumentation for the High School Laboratory". The chemical educators' discussion group has been invited to the instrumental lab of Richard Barnes at Raymond Walters College on Monday, March 3<sup>rd</sup> to explore analytical methods applicable to the high school curriculum. We will meet in room 100 of the

Science and Allied Health Building (SAHB) at 6:30 PM for light refreshments, social time, and brief announcements. Then we will head up to room 356 for sample preparation and room 362 for instrumental analysis. We will be introduced to fatty acid composition of commercial fats and oils using gas chromatography and mass spectroscopy. We will use atomic absorption to measure metal content in vitamin tablets. Please join us for this wonderful opportunity.

**Directions to Raymond Walters College:** Using either I75 or I71, travel to Ronald Reagan Highway. Go east from 75 (or west from 71) to the Plainfield Road exit. Turn left at the end of the exit onto Plainfield Road. As you travel north, Plainfield Road becomes Reed Hartman Highway at the 3<sup>rd</sup> traffic light. Bear to the left at this fork and travel one more mile to the campus located on Plainfield Road. As you enter the main entrance, the science building is ahead and to the right. Park in a white-lined stall and enter the SAHB at the east door that faces Plainfield Road. Proceed down the hall to room 100. If you arrive after 7 PM, join us up on the 3<sup>rd</sup> floor. There are nice maps and additional directions at the college website: <http://www.rwc.uc.edu/maps>.

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the recipient of a National Science Foundation postdoctoral fellowship (1988-1990), an American Cancer Society Junior Faculty Research Award (1996-1998), a WSU College of Pharmacy and Allied Health Professions Excellence in Teaching Award (1997), and a Wayne State University Career Development Award (1999). Dr. Gibbs' research interests center on the mechanisms of lipid modification of proteins, and the development of inhibitors of these processes as potential novel anticancer agents.

## The ACS Committee on Chemists with Disabilities

announces the latest edition of

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Stanley N. Deming, Stephen L. Morgan, Instructors

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- Develop a firm foundation for understanding advanced design techniques
- Receive a brief introduction to Taguchi methods
- Learn about commercial software packages for data treatment
- Improve your skills in communicating research strategies to co-workers

**About the Instructors**

**Stanley N. Deming** is Professor Emeritus of Chemistry at the University of Houston, Texas. He is also the President of Statistical Designs, a firm that offers short courses and consulting in methods development, process optimization, statistical experimental design, and the statistical analysis of laboratory data. Dr. Deming is the author or co-author of more than 90 publications in the areas of analytical chemistry and related disciplines. He is co-author (with Dr. Morgan) of the Elsevier text, *Experimental Design: A Chemometric Approach*, 2nd edition (1992).

**Stephen L. Morgan** is Professor of Chemistry at the University of South Carolina. His current research inter-

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## 2002-2003 National Chemistry Week (NCW) Poster Contest “The Chemistry of Cleaning” Winners Announced

A contest for students in grade levels, K-2, 3-5, 6-8, 9-12 in the Cincinnati tri-state area (Southwest Ohio, Northern Kentucky, and Southeastern Indiana) was held again this year. Over the past 15 years, 800 NCW chemistry contest kits were distributed each year to elementary schools, scout troops and anywhere that children can come into contact with the concept that “Chemistry is Fun”! The contest kits contained a letter to the educators, a copy of the rules, and the contest materials. This year we entered the computer age. The contest rules were sent wide and far via e-mail. We do not know how many teachers were contacted in total but we know that it was far more than the potential 800 of past years when we physical mailed out or hand delivered actual contest kits. A special thanks goes to Gwen Baumann for a yeoman’s effort in helping with the e-mail distribution process.

This year we challenged students to create a poster depicting “The Chemistry of Cleaning”. The contest rules were consistent with the rules of the National ACS Chemistry of Cleaning poster contest for NCW. Our local student winners will be entered in the national Contest to represent the Cincinnati Section.

The fact that so many individual students and teachers find time to include our contest in their busy schedule tells us how important the opportunity to be involved in this contest tradition is to them. Many teachers incorporate the contest into their lesson plans.

At one of our Teacher’s Award Night Dinner Meetings the principal of one of our contest winning schools praised the Cincinnati Section of the ACS, for our long and sustained effort to value our local educators with our NCW programs and our teacher of the Year Awards for science teachers at the elementary, middle and high school levels. He acknowledged the Cincinnati ACS Section as one of the few local organizations that consistently support local teachers and education. We continue that tradition as we prepare to honor our NCW contest winners again this year. They are:

<u>Grade Level</u>	<u>Student</u>	<u>School</u>	<u>Teacher</u>
K – 2nd grade	Alec Burris	Taylor Mill Elem. Covington, KY	Ms. Brock
3rd – 5th grade	Jonas Stalyga	Fairview German Language, Cinc.	Mrs. Skidmore
6th – 8th grade	Marvin Davis	Hays-Porter-Washburn, Cinc.	Mrs. Stargel-Harden
9th – 12th grade	Keith Bergh	Cincinnati Hills Christian Academy	Dr. Laughlin

Local Winners will be entered in national ACS Contest. National entries will be judged based upon:

- Originality and Creativity
- Relevance to and incorporation of theme
- Visual Impact and Neatness

Winners of the Cincinnati Section of the ACS along with their teachers and parents will be honored as guests of our local section’s dinner meeting, April 9, 2003, at Northern Kentucky University. The Cincinnati Section ACS will submit the local winning poster in each grade category to the National ACS Office of Community Activities. All winning posters will be displayed during the 225th ACS national meeting in New Orleans, LA, March 23-27, 2003. The National ACS Judging Committee will select one winner and one honorable mention for each grade category during the New Orleans ACS meeting for National recognition.

American Chemical Society, Cincinnati Section  
Richard Sunberg, Contest Committee Chair

(Continued from page 6)

ests include optimization and experimental design in chemistry, pattern recognition on chemical information, and data preprocessing strategies. Additional research in his laboratory involves the application of computers in chemistry, experimental design, and multivariate statistics. Dr. Morgan is the author of more than 100 publications in the field of analytical chemistry and analytical biochemistry. He and Dr. Deming have co-authored (with F. H. Walters and L. R. Parker, Jr.) , Sequential Simplex Optimization (CRC Press, 1991).

Fees will depend on the number of participants, **but are guaranteed to be significantly less than what you would pay at a National meeting or Pittcon (\$1,345 ACS members, \$1,445 non-members)**. Course seating will be limited, so indicate your interest now and be among the first to receive the final announcement, fees and registration details. Send an e-mail with your name, company, and telephone to white.dr.2@pg.com.

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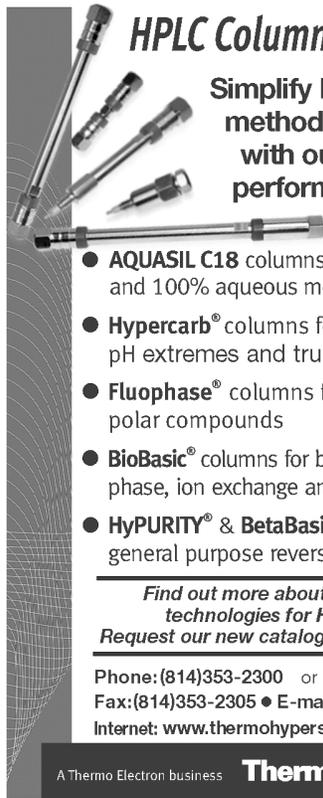
## Candidates Sought for Section Offices

The Nominating Committee is seeking nominations for the several offices for the section. We intend to have nominations completed by the March Meeting, with nominations from the floor at that point, and elections held in April, results at the May party night.

If you'd like to run or know someone who would like to run for an office, please advise Hank Greeb, ([hgreeb@one.net](mailto:hgreeb@one.net)) or 513-385-8363. We'd like willing volunteers, but will resort to arm twisting, bribery, and other nefarious acts if necessary to fill the slates of officers.

Thanks for your help with this important matter.

Hank Greeb  
Chair, Nominating Committee



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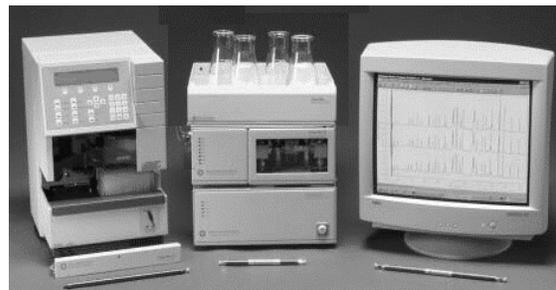


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## Travel Awards for Chemists with Disabilities Announced!

The ACS Committee on Chemists with Disabilities announces a new travel grant program. The program is open for all individuals with disabilities that are graduate, undergraduate students, or postdoctoral researchers who wish to make presentations at scientific meetings. The intent of the grant is to help defray some of the costs associated with travel and lodging. The goal of the program is to promote presentation of scientific research by individuals with disabilities and provide motivated students with opportunities to build professional relationships through networking.

The deadline for applications is March 15, 2003 for meetings scheduled between July 1 and December 31, 2003. For further information, please go to <http://membership.acs.org/C/CWD//travap> or contact Kathleen Thompson 800-227-5558 ext.

### A THOUGHT TO PONDER....

*When you counsel someone, you should appear to be reminding him of something he had forgotten, not of the light he was unable to see.*

--Baltasar Gracian

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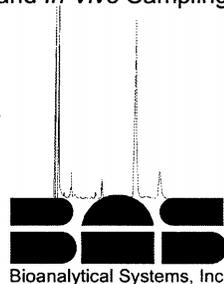
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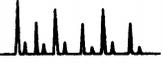
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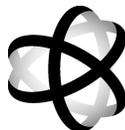
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