



# The TarHelium

Volume 24, Number 6

February 1994

## Polymer Discussion Group

Thursday, February 10, 1994

Andrew Woo  
Reichold Chemicals

"Rheological Behavior of Abrasion-Resistant, Self Healing Polyurethane Coatings"

NCSU Faculty Club  
4200 Hillsborough St., Raleigh

5:30 p. m. Social Hour

6:30 p. m. Dinner† (members-guests:  
\$15; students \$8)

7:30 p. m. Lecture

†Reservations by noon, February 8, with  
Walter Pawlowski (919) 543-2243 (IBM-  
RTP).

## 11<sup>th</sup> Annual TCDG Symposium and Instrument Exhibit

The Triangle Chromatography Discussion Group (TCDG) will hold its 11<sup>th</sup> Annual Exhibit, Symposium and Poster Session at the McKimmon Center in Raleigh on Thursday, May 19, 1994. As part of this meeting, the Group will sponsor a poster session. Anyone is invited to participate in the poster session, but for student posters only, prizes will be given. The first prize is \$400 and second prize is \$200. Deadline for receipt of abstracts is Friday, April 1, 1994. The abstract should be no longer than one page. Send the abstract along with title, authors, affiliation and complete address and phone number to:

Dr. Joe Hudson  
Rhône-Poulenc Ag Company  
P. O. Box 12014  
Research Triangle Park NC 27709

Acceptance will be acknowledged no later than the end of April 15, 1994.

## 108<sup>th</sup> NC Section Conference

The 108<sup>th</sup> Conference of the North Carolina Section is planned for Saturday, April 16, 1994 at Duke this year. Please join us in presenting papers at this meeting. It is run as closely as possible to the format of a national meeting. There is an opportunity to present in either a regular or a poster session. As in past years, we plan to have a meeting favor for those who present and we invite all presenters to be the guest of the Section at a buffet luncheon that follows the meeting. The deadline for receipt of titles is Friday, March 11, 1994. An application form showing the required information is given in the Call for Papers on Page 2. Please feel free, however, to send the information by e-mail, FAX or phone.

### The TarHelium

c/o William L. Switzer, Editor  
Department of Chemistry-8204  
North Carolina State University  
Raleigh NC 27695-8204

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M. T. Riebe (Glaxo), Chair Elect  
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**Voicemail Information Line:** (919) 541-7183 in the RTP

10-General ACS  
11-Polymer Discussion Group  
52-NMR Discussion Group  
53-Mass Spectrometry Discussion Group  
54-Triange Chromatography Discussion Group

#### National ACS meetings:

March 13-18, 1994, San Diego  
August 21-26, 1994, Washington  
April 2-7, 1995, Anaheim  
August 20-25, 1995, Chicago  
March 24-29, 1996, Seattle  
August 25-30, 1996, Boston

**Deadline for March Publication: February 1, 1994**

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W. L. Switzer, Editor  
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*The TarHelium* is a publication of the North Carolina Section of the American Chemical Society. The views expressed herein are not necessarily those of the Section. Public lectures and seminars as well as announcements of interest to the ACS membership will be listed as deemed appropriate by the editor and as space permits. Short commentaries or contributed articles will also be considered. Also, we are happy to publicize, free of charge, any job openings for chemists. (We also accept paid advertisements for more extensive recruiting announcements.) The **Deadline** for each publication is usually the first of the month prior to publication.

Contributions for *The TarHelium*: Send to W. L. Switzer, Editor, Chemistry-8204, North Carolina State University, Raleigh NC 27695-8204. Phone: (919) 515-2945, Fax: (919) 515-5079 and Internet: bill\_switzer@ncsu.edu.

**Advertising:** All nine issues of the *TarHelium* will accept advertising. The cost is: \$25 per column-inch based on a 3.5 inch width; two-inch minimum. There is a 10% discount for advertising in four or more issues in a publication year which runs from September through April plus one issue in the summer. Contact Paul Flowers, Advertising Manager, Department of Physical Science, Pembroke State University, Pembroke NC 28372, Phone: (919) 521-6247 Fax: (919) 521-6649 and Internet: paul@nat.pembroke.edu.

Donations to the NC Section of the ACS help sustain Local Section activities. All contributions are tax deductible and greatly appreciated.

If you wish to change your membership status or *The TarHelium* mailing address, please submit your new address along with your old address in the form of a recent *C&EN* or *TarHelium* address label to:

Manager, Membership & Subscription Services  
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P. O. Box 3337  
Columbus, OH 43210

If you wish to receive announcements of Local Section ACS events by electronic mail, please submit your e-mail address to the Internet address given above for the Editor.

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## CALL FOR PAPERS

**108<sup>th</sup> NC Section Conference**  
**Saturday, April 16, 1994**  
**Duke University, Durham NC**

Author(s): \_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

Position(s): \_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

Title: \_\_\_\_\_

Phone (senior author): \_\_\_\_\_

e-mail address: \_\_\_\_\_

Presenter: \_\_\_\_\_

Institution: \_\_\_\_\_

Session:

Analytical       Biochemistry       Chemical Education

Inorganic       Organic       Physical

Polymer       Other

Other (specify):

Type of Session:     Regular       Poster       Either

Type of Projector: \_\_\_\_\_

**DEADLINE: Friday, March 11, 1994**

**Send application to:**

William L. Switzer      Internet: bill\_switzer@ncsu.edu  
Chemistry-8204      (919) 515-5079 (FAX)  
North Carolina State University      (919) 515-2945 (W)  
Raleigh NC 27695-8204      (919) 217-9095 (H)

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## Job Openings

All job announcements are broadcast immediately upon receipt to the e-mail distribution list. If you wish to be included send your address to: [bill\\_switzer@ncsu.edu](mailto:bill_switzer@ncsu.edu).

**Burroughs Wellcome:** Job Line at (919) 315-8347.

**EPA-RTP:** Job line (919) 541-3014. Updated every Friday.

**Glaxo:** Job Line (919) 248-2565.

**RTI:** Contact: Research Triangle Institute, Office of Human Resources, PO Box 12194, Research Triangle Park NC 27709-2194. Phone: (919) 541-6466. Analytical Chemist I G0077 76A BA/BS in Chemistry with experience or training in analytical instrumentation. Class 100 clean room and trace metal experience is preferred. Will operate Gas Furnace AA and ICP, prepare samples for instrumental analysis. work with spreadsheets. Analytical Chemist I G0078 76A BA/BS in Chemistry with experience or training in analytical instrumentation. Class 100 clean room and trace metal experience is preferred. Will operate Gas Furnace AA and ICP, prepare samples for instrumental analysis, work with spreadsheet. Chemist I F0415 63A BS in Chemistry with training or experience in organic synthesis. Will synthesize, purify and analyze organic compounds. Chemist I F0431 63A BS/BA in Chemistry with training in organic synthesis. Will synthesize novel organic compounds. Chemist I F0432 63A BS/BA in Chemistry with training in organic synthesis. Will synthesize novel organic compounds. Chemist I/II F0427 63A BS/BA in Chemistry with emphasis in organic chem-

istry and training or experience in analytical methods. Will conduct studies of the metabolism of drugs and environmental chemicals and analyze biological fluids for these chemicals. Natural Products Scientist F0437 60A PhD with research experience in the isolation, structure determination, synthesis, or testing of natural products. Will lead natural products research, write successful grant/contract proposals, manage research projects and supervise laboratory staff. Postdoctoral Chemical Engineer J0255 96A PhD in Chemical Engineering with experience in gas-solid reactions and catalysis or fluid bed reactors. A background in gas separation is desirable. Will construct and operate bench-scale desulfurization/sulfur recovery reactor systems; analyze data; write technical reports and publications. Postdoctoral Chemist F0417 60A PhD in Organic Chemistry with synthetic chemistry research experience. Will synthesize phosphonates and protein conjugates with some metabolism and kinetics work possible. Postdoctoral Chemist F0422 63A PhD in Chemistry with research experience in organic synthesis. Will conduct research in the synthesis of organic compounds. Postdoctoral Chemist F0423 63A PhD in Organic Chemistry. Duties include organic synthesis. Postdoctoral Chemist F0424 63A PhD in Organic Chemistry plus experience with organic synthesis. Duties include radiosynthesis. Postdoctoral Chemist F0426 63A PhD in Chemistry with experience in organic synthesis. Will synthesize novel organic compounds. Postdoctoral Chemist F0428 64A PhD in biochemistry, molecular biology or related biological science. Background in biochemistry, enzymology or cell biology is required. Experience with radiolabeled tracer techniques is desired. Will conduct research to develop mechanistic-based assays for anti-cancer agents found in natural products, particularly plants. Postdoctoral Chemist F0429 64A PhD in organic chemistry with experience or training in organic synthesis. Will conduct research to synthesize novel organic compounds. Postdoctoral Chemist F0430 63A PhD in Organic Chemistry with training in organic synthesis. Will conduct research to synthesize novel organic compounds. Postdoctoral Chemist F0433 60A PhD in Chemistry with training in organic chemistry. Will synthesize haptens and conjugates for catalytic antibody programs. Will involve some analytical (kinetics) work. Postdoctoral Chemist F0435 63A PhD in Organic Chemistry with research experience in organic synthesis. Will conduct research on the synthesis of novel organic compounds. Postdoctoral Chemist F0436 63A PhD in Chemistry with research experience in organic synthesis. Will synthesize novel organic compounds. Postdoctoral Chemist F0438 63A PhD in chemistry with research experience in organic synthesis. Will synthesize novel organic compounds. Res. Analytical Chemist II/III G0071 72A PhD in Analytical Chemistry with 2-5 years of experience in analytical/environmental chemistry. Experience conducting independent research programs. Should have good communication and management skills, develop independent research programs, write proposals and grants, manage projects, interact with clients. Research Associate I J0254 72A PhD in chemical Engineering with 2-3 years experience in gas-solid reactions and catalysis or fluid-bed reactors. A background in gas separation is desirable. Will construct and operate bench-scale desulfurization/sulfur recovery reactor systems; analyze data; write technical reports and publications.

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## Area Seminars

- Feb 4 J. J. Hren, North Carolina State University, "Vacuum Microelectronics: Materials Science at Nanometer Dimensions", Duke
- Feb 7 Mark Wightman, University of North Carolina, Chapel Hill, "Electrochemistry at a Single Cell", NCSU
- Feb 9 R. N. Zare, Stanford University, "Reactions a la Mode", Peter Smith Lecture, Duke
- Feb 10 Andrew Woo, Reichold Chemicals, "Rheological Behavior of Abrasion-resistant, self healing polyurethane coatings", Polymer
- Feb 11 L. G. Marzilli, Emory University, "NMR Studies of Pt Anticancer Drug-DNA Interactions", Duke
- Feb 14 Sandra Greer, University of Maryland, "Structure and Properties of Living Polymer Solutions", NCSU
- Feb 17 E. Ehrenfeld, University of California, Irvine, "Polio Virus Replication", NCSU-BC, Glaxo

Polymer-Polymer Discussion Group. Call Walter Pawlowski 543-2243 (IBM-RTP). Voice Mail 541-7183, box 11 Duke (Chemistry) Call Bonnie Turner at 660-1506. NCSU (Chemistry) Call Joyce Weatherspoon at 515-2548. NCSU-BC (Biochemistry) Call Pat Sullivan 515-2581.

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## Area News

**Boron Biologicals:** Building upon an earlier, multi-year research contract and licensing agreement, Guerbet S.A., a French pharmaceutical and diagnostics company, has made a substantial equity investment in Boron Biologicals Inc. (BBI). Under the terms of the earlier multi-year research contract and licensing agreement, BBI designs, synthesizes and characterizes new con-

trast agents. A contrast agent is a radiopaque substance that is injected into the body to help visualize internal organs in X-ray imaging. Guerbet provides initial testing and selection of the new compounds and subsequent clinical testing and development. Patents resulting from the compound development effort will be owned jointly by BBI and Guerbet. Guerbet will receive exclusive marketing and distribution rights to these compounds.

BBI has also recently moved to a new location in Raleigh, N.C., tripling its previous space. All laboratories and manufacturing facilities are now consolidated in one location. The new location will allow BBI to establish a Good Manufacturing Practices (GMP) facility.

**Duke:** Chemistry Professor **Charles H. Lochmüller** has had a cooperative research program with the Chemistry Institute of the Estonian Academy of Sciences for almost a decade. The liberation of Estonia following the fall of the USSR has left science and scientists without many needed resources. Professor Lochmüller has written proposals and received some \$35,000 in ACS journal subscriptions for the Academy Library. With the help of individuals and the Biddle Foundation, he has just shipped some \$750,000 more in reference and bound journal gifts to Tartu University in Estonia. Tartu was the home of Ostwald the Nobel Laureate and, of course, Tswett the inventor of chromatography. American Veneer of Beaufort, NC is carrying the two tons of books in four crates which contain among others a full, current run of Beilstein to Tartu along with equipment for a plant they are constructing nearby.

**Charles H. Lochmüller** also has been invited to lecture at the University of Helsinki this summer for the 5th Nordic Summer School in Polymer Chemistry. His lectures will be focused on chemometric methods and their use in studying complex chemical reactions. The program, which runs from August 22-26, deals with Polymer Degradation and Stabilization. Sessions topics include Biodegradable Polymers Synthesis, Degradation and Stabilization of Synthetic Polymers, and Methods of Thermal Analysis.

**NCSU:** At its fall graduation ceremonies, NCSU Chemistry recognized 12 graduates with the BS degrees in Chemistry and 32 with the BA degrees. **Joshua Ethan Malinsky**, Hummelstown PA was recognized as the recipient of the 1993 Research Award given by the College of Physical and Mathematical Sciences. The ceremony also recognized 8 recipients of BA degrees in Chemistry following the first summers session and 5 recipients of BA degrees following the second summer session.

**Sphinx:** Sphinx Pharmaceuticals Corporation announced that, as of December 1, 1993, Richard W. Reichow will serve as interim President and CEO following the departure of Clayton I. Duncan, who tendered his resignation effective November 30. Mr. Reichow has been involved with Sphinx since its first venture financing in 1988 and has served as the Company's Vice President of Finance and Administration since 1991 and as Chief Financial Officer and Treasurer since 1990.

Also Sphinx announced that it has initiated a Phase I clinical trial of Kynacyte<sup>®</sup> (safingol) to determine the safety and pharmacokinetics of the compound when administered intravenously alone and in combination with doxorubicin, a commonly used anticancer drug. The Phase I dose-escalating trial will be conducted under the supervision of Gary Schwartz, M.D. at Memorial Sloan-Kettering Cancer Center in New York City, and is intended to enroll 20 to 30 cancer patients.

Kynacyte is a compound that inhibits the activity of a family of intracellular enzymes known as protein kinase C (PKC), which is required for various cellular processes that support the growth and spread of cancer. By inhibiting PKC, the effects of conventional anticancer drug therapy may be enhanced. In preclinical studies with cancer cells and other tumor test systems, Kynacyte has been shown to enhance the antiproliferative effects of doxorubicin and to potentiate doxorubicin's ability to suppress tumor growth.

### From the National ACS Office

- A report, "An Analysis of Funding for Academic R&D in the Chemical Sciences at the National Institutes of Health FY 1982 to FY 1991," published this month by the American Chemical Society examines the extent of federal funding of the chemical sciences by NIH. Copies of the report can be obtained from the ACS Department of Government Relations and Science Policy, at 202/452-2127. The ACS report finds that "the chemical sciences were direct beneficiaries of NIH's dramatic growth during the 1980's." The report quantifies NIH's support for the chemical sciences as a percentage of all federal support.

- More than 9,000 proposals originating in former Soviet Union (fSU) countries will be judged during December in a large peer review exercise involving the American Chemical Society (ACS), the International Science Foundation (ISF) and other major scientific societies.

- The 'Chemistry in Context' program for college students exposes non-science majors to chemistry. College students who aren't majoring in science still can benefit from a grounding in the subject. *Chemistry in Context: Applying Chemistry to Society*, a new textbook and accompanying laboratory manual made its commercial debut on November 19, 1993. The text fills this need by showing undergraduates how science affects them and their environment. The program is designed to enhance their understanding of science issues that have an impact on their lives as consumers and citizens. The one-semester program has been tested in preliminary form by 1,500 students at 19 universities, colleges and community colleges around the country, including Lehigh University, Bethlehem, PA; Johnson C. Smith University, Charlotte, NC and Lakewood Community College, White Bear Lake, MN. The text is published by the ACS and Wm. C. Brown Publishers. The textbook will be available to students for about \$43, and the lab manual will cost about \$19. To order a copy, please contact Wm. C. Brown's Educational Services Department at (800) 228-0459.

### Housing at ACS Meetings

Looking for a roommate for an ACS meeting? Why not advertise in The TarHelium. Send us your name, gender, preference for smoking/nonsmoking, address, daytime/evening telephone number, and for which ACS meeting(s) you are seeking a roommate. We will publish this information in our newsletter under a roommate wanted ad and members can help each other find roommates. We will not take responsibility for roommate matches.

## Four Day Workshop at MCNC

### INTRODUCTION TO GAUSSIAN: THEORY AND PRACTICE

April 26-29, 1994

The North Carolina Supercomputing Center and Gaussian Inc.

MCNC

North Carolina Supercomputing Center  
3021 Cornwallis Road

Research Triangle Park, NC 27709-2889

The NC Supercomputing Center (NCSC) is pleased to offer "Introduction to Gaussian: Theory and Practice." This four day workshop will be presented in conjunction with Gaussian, Inc., on April 26-29, 1994 at NCSC in Research Triangle Park, NC.

The workshop provides an overview of the Gaussian software package and introduces participants to electronic structure methods. This workshop will also provide an excellent review for researchers active in the field. Attendance is open to researchers at all levels of academic, government and industrial research.

Gaussian 92/DFT is a user-friendly set of programs for performing *ab initio*, density functional, and semi-empirical molecular orbital calculations. This workshop provides an introduction to the underlying theory along with practical pointers. All of the *ab initio* and density functional methods available in Gaussian 92 will be covered, along with discussion on choosing methods appropriate to the chemistry being studied. Additional topics will include estimating computer resource requirements and dealing with computational difficulties.

#### INSTRUCTORS:

Dr. Michael J. Frisch	Lorentzian, Inc.
Prof. H. Bernard Schlegel	Wayne State University
Prof. John A. Pople	Northwestern University
Dr. Douglas J. Fox	Gaussian, Inc.

AGENDA: •Building Gaussian Input Decks; •Model Chemistries (basis sets, level of theory); •SCF Methods (RHF/UHF/ROHF, GVB, MCSCF); •Stability and Convergence of SCF Wavefunctions; •Geometry Optimization: Techniques for Finding Energy Minima; •Studying Transition States: Optimization and Reaction Paths; •Electron Correlation Methods; •Excited States via CI Singles; •Interpretation of Results and Molecular Properties o Solvent Effects on Molecular Electronic Structure; •Gaussian Utilities; •Guidelines for Choosing Algorithms and Estimating Resources; •Density Functional Methods

TRAINING MATERIALS: There will be hands-on sessions each day between the morning and afternoon lectures. Additional hands-on sessions will be available until the building closes at 5:00pm. Workshop participants will be provided with a class computer account, of limited allocation, on NCSC's CRAY Y-MP for use during the hands-on workshop sessions. Each workshop participant will also be provided a copy of the lecture notes, a copy of the Gaussian 92 User's Guide, and a copy of "Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian."

THE TRAINING FACILITY: Our training facility has 15 DEC Alpha AXP (OSF/1) workstations equipped with color monitors for state of the art graphics training. The number of students must be limited to allow adequate training to all attendees.

GAUSSIAN 92/DFT AVAILABILITY: Gaussian software is available on our CRAY Y-MP supercomputer to North Carolina

academic and licensed commercial users. For account information, people from North Carolina academic institutions should send electronic mail to <info@mcnc.org> to request account information; interested corporate users should contact our Business Development Office at 919-248-1133.

REGISTRATION: Registration is first-come-first-served based upon receipt of payment and the completed registration form. Please fill out a separate form for each attendee and mail it to

MCNC--Gaussian Workshop  
 North Carolina Supercomputing Program  
 Attn: Course Registrar  
 P.O. Box 12889  
 3021 Cornwallis Road  
 Research Triangle Park, NC 27709-2889

Cancellations must be made at least 2 weeks prior to course starting date to receive a refund. Hotel selections will be mailed to conference participants. Hotel, travel, and meals are at the separate expense of participants, except for lunches and refreshments which will be provided.

DEADLINES:

Receipt of Registration Materials:	March 25, 1994
Receipt of Registration Fee:	April 8, 1994
Receipt of Cancellations to receive refund:	April 15, 1994
Receipt of Notification of Substitution:	April 22, 1994

REGISTRATION FEE:

\$1,400 General Registration  
 \$1,200 Government or Nonprofit Organization  
 \$1,200 MCNC Partner\* and For-Profit Company  
 \$1,000 MCNC Partner\* and Government/Nonprofit Organization  
 \$150 Academic

\*Attendees employed and enrolled by a company having a partnership agreement with MCNC. This includes sponsors of the IAC, Supercomputing Collaborative Research Partnerships, and MCNC affiliated companies.

REGISTRATION FORM:

Name: \_\_\_\_\_

Affiliation: \_\_\_\_\_

Address: \_\_\_\_\_

\_\_\_\_\_

Telephone: \_\_\_\_\_

Facsimile: \_\_\_\_\_

E-Mail Address: \_\_\_\_\_

Please indicate your Research Status (check one):

Faculty;  University Research Staff;  University Non-Research Staff; Student:  Undergraduate;  Graduate;  Postdoctorate;  Government;  Industrial

Other \_\_\_\_\_

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