

THE

TarHelium



A Publication of the North Carolina Section of the American Chemical Society

Vol. 17, No. 7

March 1987

Some Graphics Tools for Molecular Structures

*A lecture illustrated with videotapes and
followed by live demonstrations by*

Dr. Frederick P. Brooks

Computer Science Department

University of North Carolina — Chapel Hill

Tuesday, March 17, 1987

University of North Carolina — Chapel Hill

Sponsored by

North Carolina Section, ACS

- Social Hour:* 5:30 p.m. Jade Palace, Carrboro
- Dinner:* 6:30 p.m. Jade Palace, Carrboro
\$12.00 members/guests; \$6.00 students
- Lecture:* 8:00 P.M. 265 Phillips Hall (Physics Building),
UNC—Chapel Hill

What is a Chemist Today?*

A Lecture by

Dr. Mary L. Good

President, American Chemical Society, 1987

President, Engineered Materials Research, Allied-Signal, Inc.

Wednesday, March 25, 1987

University of North Carolina — Chapel Hill

Sponsored by

North Carolina Section, ACS

- Social Hour:* 5:30 p.m. Carolina Inn, Chapel Hill
- Dinner:* 6:30 p.m. Carolina Inn, Chapel Hill
\$14.00 members/guests; \$7.00 students
- Lecture:* 7:30 P.M. 207 Venable Hall, UNC—Chapel Hill

(See inside for directions to both meeting and dinner locations)

Members and guests are welcome at both the lecture and dinner; however, if attending either dinner, please make reservations by 5:00 p.m. Friday, March 13 for the March 17 meeting and by Friday, March 20 for the March 25 meeting. In Chapel Hill call Debbie Edwards at 962-2172; in Durham call Earlene Beamon at 684-2414; in Raleigh call Joyce Dunn at 737-2545; in Fayetteville call Sandra Smith at 486-1500. To cancel reservations, please call Joyce Dunn in Raleigh at 737-2545.

*Rescheduled from Feb. 18 date, which had been canceled due to inclement weather.

Mary L. Good

President, American Chemical Society

President, Engineered Materials Research, Allied-Signal Inc.

Mary Good was born in Grapevine, Texas, in 1931 and grew up in Arkansas. She graduated from the Arkansas State Teachers College (now the University of Central Arkansas) in 1950 with a B.S. in Chemistry and the highest scholastic standing in her class. In graduate school at the University of Arkansas Fayetteville, she majored in inorganic and radiochemistry, earning a M.S. in 1952 and a Ph.D. in 1954.

She began her professional career as instructor of chemistry at Louisiana State University (LSU) at Baton Rouge in 1954 and became full professor at the University of New Orleans in 1963. She served as Boyd Professor of Chemistry at the University of New Orleans, 1974-78, and Boyd Professor of Materials Science at LSU-Baton Rouge, 1978-80.

In 1980, Dr. Good took an industrial position as Vice President and Director of Research with UOP Inc. Since then, she has led the transition to corporate research center for the Signal Companies and now to Allied-Signal's Engineered Materials Research Center. She broadened and deepened the center's research capabilities, developing major programs in materials science, biotechnology, separations science, and materials-by-design.

Her research interests include spectroscopic techniques applied to materials characterization; solid state and surface chemistry; characterization of the chemical, physical, and environmental properties of anti-fouling marine coatings containing organometallic toxicants; marine corrosion; preparation and characterization of transition metal complexes that exhibit low dimensional magnetic properties; and complex chemistry of ruthenium and the characterization of supported ruthenium catalysts.

Dr. Good has authored approximately 100 articles in refereed technical journals, several publications on science policy and research strategy, and one book. A recipient of the ACS Garvan Medal, Dr. Good has held many local and national ACS offices and has served on numerous advisory committees and editorial boards.

What is a Chemist Today?

In these days of rapidly changing technology, scientists trained as chemists are choosing to work in non-traditional new fields such as materials science and biotechnology. We call them genetic engineers, molecular biologists, chemical biologists, chemical physicists, and materials designers. What does this mean for the future of chemistry: research opportunities, education, and public perception?

Actually, the distinctions are not new. There are simply many more of them. Chemistry has never been separate from the rest of science. Our

classifications have become more precise as our technologies have grown more diverse and sophisticated. The secret is in how to participate in new, exciting research areas using the same old essential skills of chemistry combined with the new molecular skills to make programs go. Materials-by-design is a good example of how the chemist fits into the new technology.

Dr. Frederick P. Brooks, Jr.

Dr. Frederick P. Brooks, Jr. is Kenan Professor of Computer Science at the University of North Carolina in Chapel Hill. He is best known as the "father of the IBM System/360 computer family," having served as Project Manager for the hardware and later as Project Manager for the Operating System/360 software. Earlier, he was an architect of the IBM Stretch and Harvest computers. A native of North Carolina, Dr. Brooks received his A.B. at Duke and M.S. and Ph.D. (in what is today Computer Science) from Harvard, where he was a student of Howard Aiken.

At Chapel Hill, Dr. Brooks founded the UNC Department of Computer Science and has participated in the establishment and guiding of the Microelectronics Center of North Carolina, the Triangle Universities Computation Center and the North Carolina Educational Computing Service. He has published technical papers and book chapters and *Automatic Data Processing* (co-authored with Kenneth Iverson). His best known work is *The Mythical Man-Month: Essays on Software Engineering*. He is a member of the National Academy of Engineering, the American Academy of Arts and Sciences, and the Defense Science Board. He has received the National Medal of Technology, a Guggenheim Fellowship and the IEEE Computer Society's McDowell and Computer Pioneer awards.

Some Graphics Tools for Molecular Structures

Since 1970 our graphics research group has built experimental hardware/software systems for visualizing macromolecules, collaborating with several teams of molecular scientists. The first protein structure to be determined with the aid of computer graphics instead of a brass model was solved by our GRIP team. Another graphic system, GRINCH, provides a new way of doing *ab initio* interpretation of electron-density maps determined by x-ray crystallography.

Current work emphasizes the docking of small molecules into active sites. An experimental system provides a force display with which the scientist can feel the electron force fields. Other visualization systems are also aimed at this problem. Another thrust of our current work is the development of entirely new 3-D, dynamically movable visualizations of molecular and electron densities. The talk will be illustrated with videotapes and followed by live demonstrations.

DIRECTIONS TO THE MARCH DINNERS AND MEETINGS

March 17 Meeting

The social hour and dinner are being held at the Jade Palace in Carrboro. Take Rosemary Street, which is 1 block north of Franklin, from Chapel Hill to Main Street in Carrboro. Just past railroad track, take the 'Y' to the left to continue on Main Street. The Jade Palace is located on the north side of the street in the first block after the 'Y'. The meeting will be held in room 265 Phillips Hall, which is across the parking lot from Venable Hall. The best parking is at the pay parking lots just off Rosmary Street near the intersection with Columbia in Chapel Hill.

March 25 Meeting

From Raleigh, take Highway 54 west to Chapel Hill. From Durham, take US 15/501 to Highway 54 in Chapel Hill; turn heading west. Immediately after passing Kenan Laboratory on the right, Highway 54 will turn right. The Carolina Inn is located immediately on the left and Venable Hall on the right.

DR. HERMAN F. MARK SPEAKS TO POLYMER GROUP ON APRIL 2, 1987

The Polymer Group will meet at the North Carolina State University Faculty Club on Thursday, April 2, 1987. The speaker will be Professor Herman F. Mark from the New York Polytechnical Institute. The title of his presentation is "Recent Advances in Textile Science." Born in Austria in 1895, Dr. Mark began working with polymers in 1921. Dr. Mark has authored more than 500 papers in the area and is recognized as one of the dominant contributors to the development of polymer science. The Polymer Group is honored to have such a distinguished speaker and invites all to attend. Reservations are not necessary for the talk at 7:30, but are requested for the social hour and buffet dinner at 5:30 and 6:30 respectively. Call Dr. Ray Kirby at 543-8043 or Dr. Fred Robinson at 469-6760. The NCSU Faculty Club is located on Hillsborough Street between the Raleigh Beltline and the NC State Fairgrounds.

PROFESSIONAL RELATIONS

The ACS Department of Professional Services has sent copies of its *Professional Employment Guidelines*, a flyer describing statistical services for professionals and a booklet listing employers who have had multiple terminations within the last 10 years. Anyone needing this information may contact the Chairman, William L. Switzer, Department of Chemistry-8204, North Carolina State University, Raleigh, NC 27695-8204; (919) 737-2845.

1987 MEETING-IN-MINIATURE AT DUKE

The program for the 1987 Meeting-in-Miniature at Duke is being prepared by Dr. William Hatfield. The Section is pleased to announce financial support of the following industrial organizations:

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APPLICATION

Meeting-in-Miniature
Saturday, April 11, 1987
Duke University

Author(s): _____

Phone number of senior author: _____

Position(s): _____

Presented by: _____

Institution: _____

Title of Paper: _____

Session: ___ Analytical ___ Inorganic
 ___ Biochemical ___ Organic
 ___ Chemical Education ___ Physical
 ___ Polymer ___ Other

Regular session ___ *Poster session ___ *Either session ___

Type of projector needed (if any) _____

Mail application and contact immediately: Dr. William E. Hatfield
Department of Chemistry
University of North Carolina
Chapel Hill, NC 27514
966-2296

*If enough people are interested, the poster session will be added.

PROGRAM COMPLETED FOR MAY CHROMATOGRAPHY SYMPOSIUM

On Thursday, May 14, 1987 the Triangle Chromatography Discussion Group and the North Carolina Section of the ACS are cosponsoring the 4th Triangle Chromatography Symposium and Instrument Exhibit at the Jane S. McKimmon Center in Raleigh.

- 9:00 JAMES N. LITTLE—*Zymark Corporation*
"Robotic Sample Preparation for GC and HPLC"
- 9:45 Coffee Break—Instrument Exhibit
- 10:30 THOMAS E. BEESLEY—*Advanced Separation Technologies Inc.*
"Application of Bonded Cyclodextrins for the Separation of Various Isomers"
- 11:15 R.K. GILPIN—*Kent State University*
"Surface Chemistry of Bonded Materials"
- 12:00 Luncheon at the McKimmon Center—Instrument Exhibit
- 1:30 KENNETH WILSON—*Applied Biosystems*
"Microbore and Narrow Bore Separations of Proteins and Polypeptides"
- 2:15 JOHN W. DOLAN—*LC Resources Inc.*
"Expert Systems in HPLC"
- 3:00 Coffee Break—Instrument Exhibit
- 3:45 MILTON L. LEE—*Brigham Young Univ. and Lee Scientific*
"Current Trends in Capillary Supercritical Fluid Chromatography"
- 4:30 MARVIN VESTAL—*Vestec, Inc.*
"HPLC-Mass Spec Interfaces"
- 5:15 Social Hour/Reception

SYMPOSIUM ON "STRUCTURE AND ORDER IN POLYMERS"

A symposium on "Structure and Order in Polymers" will be held on June 18-19, 1987 at Duke University to honor William R. Krigbaum, James B. Duke Professor of Chemistry, Duke University. Technical sessions will include invited presentations by A. Ciferri, University of Genoa; B. Crist, Northwestern University; J.V. Dawkins, Loughborough University of Technology; R.W. Godwin, BASF Corporation; R.J. Roe, University of Cincinnati; K.J. Smith, Syracuse University; L. Sperling, Lehigh University; I. Uematsu, Tokyo Institute of Technology. Contributed papers on polymer chemistry or polymer science are welcome: contact Professor Peter Smith, Department of Chemistry, Duke University (919/684-2238).

ONE-DAY WORKSHOP

"Analytical Gas Chromatography—Practical Capillary GC"

DR. WALTER JENNINGS

Sponsored by: The North Carolina Section, American Chemical Society
and The Triangle Chromatography Discussion Group

Date: Wednesday, May 13, 1987

Time: 9:00 am—5:00 pm

Place: Jane S. McKimmon Center, Western Blvd., Raleigh, NC

Instructor: Dr. Jennings is a professor in the Department of Food Science and Technology at the University of California at Davis and is a co-founder of J&W Scientific, Folsom, California. He is recognized as a leader in the field of capillary gas chromatography and has authored two books and many publications in that area of analytical chemistry. In the last several years, Dr. Jennings has taught over 300 workshops involving capillary gas chromatography at points all over the world.

Course Description: Based on a format designed primarily for the practicing analyst, the material is presented in such a manner that it is also valuable background for research supervisors and management personnel. The course begins with simplified considerations of the fundamentals and proceeds rapidly to state-of-the-art. Handout materials, excerpted from Professor Jennings' new book, "Analytical Gas Chromatography," which is scheduled to be released by Academic Press in August 1987, will be provided. Registrants desiring further information should contact Dr. Charles Sparacino, Research Triangle Institute, (919) 541-6581.

REGISTRATION FORM

(Registration deadline is May 5, 1987)

Enclosed is a check (payable to the NC Section, American Chemical Society) as registration fee for "Analytical Gas Chromatography—Practical Capillary GC." My cancelled check is my receipt. Proceeds support the ACS Centennial Scholarship Fund and the TCDG program fund.

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Send to: Joan Burse
Treasurer, NC Section ACS
101 Longwood Pl, Chapel Hill, NC 27514

THE CENTENNIAL SCHOLARSHIP AWARD

The North Carolina Section of the ACS announces its CENTENNIAL SCHOLARSHIP AWARDS for 1987. Up to three awards of \$500 each will be made; normally, two will be awarded to graduate students from doctoral-granting institutions and one to a student from an institution offering the master's degree or significant opportunities in research to undergraduate students. These awards will recognize achievement and potential in chemistry research and should be used to help the student further that potential.

Award Criteria include research accomplishments, excellence of academic records, and quality of the application.

Eligibility requirements are attendance at a college or university within the NC section territory and research in a department of chemistry, biochemistry, or chemical engineering.

Applications must include duplicate copies of the following:

- a summary, up to 1000 words, written by the applicant describing research accomplishments or progress,
- a letter of recommendation from the student's research director,
- a copy of the appropriate transcript(s) (graduate or undergraduate), and
- a description of how the award will be used.

Restrictions for use of the award require the student chosen to consult with his or her research advisor about how to use it.

The deadline for submitting applications is Friday, March 20, 1987. Submit applications to:

Dr. Robert W. Shaw
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

Award recipients will be announced at the Meeting-in-Miniature on April 11, 1987.

IMPLICATIONS OF THE NEW TAX LAWS

Mr. Wayne T. Stellar of Associated Financial Consultants, Inc. in Raleigh has agreed to give a one hour seminar on the implications of the new tax laws for chemists. The seminar will be held in Dreyfus Auditorium at Research Triangle Institute at 5:00 p.m., Thursday, March 26.

UNC PUBLIC HEALTH CONFERENCE

The University of North Carolina will hold its annual public health conference April 9-10 on the UNC Chapel Hill campus. Entitled, "Current Challenges for Public Health Policy," the conference will address topics such as:

Hazardous and Low-Level Radioactive Waste: Implications on North Carolina
Influencing Policy at the Federal Level
Vitamins and Minerals: Fact or Fallacy
AIDS Update: Epidemiology and Policy
Women's Issues in Public Health
School Base and Adolescent Care
Community Grass Roots: How to do Effective Outreach

The keynote speaker for the conference will be Dr. Bernard D. Goldstein, Chairman, Department of Environmental and Community Medicine, Robert Wood Johnson Medical School, Rutgers University.

For additional information concerning the conference, contact:

Harriet Barr
UNC School of Public Health
Chapel Hill, North Carolina 27514
(919) 966-3294

DR. MILOS NOVOTNY TO SPEAK

Dr. Milos Novotny from Indiana University in Bloomington will speak to the Triangle Chromatography Discussion Group (TCDG) Thursday, April 2 at the N.C. State University Faculty Club. The title of his talk is "Capillary separation methods: A key to improvements in resolution and detection capabilities." A cash bar will be available in the lounge at 5:30 p.m. A buffet dinner will be served at 6:30 p.m.; the cost of the dinner is \$9.00. The program will begin at 7:30 p.m. All interested chromatographers are encouraged to attend the lecture. Anyone interested in attending the dinner should make reservations with Dr. John Hines (RTI) at 541-6647 by Monday, March 30.

The talk will be preceded by a brief but important business meeting. At the meeting a constitution will be presented and officers will be elected. The NCSU Faculty Club is located on Hillsborough Street in Raleigh between the beltline and the N.C. State Fairgrounds. Dr. Novotny will speak earlier in the day at Glaxo. The title of his presentation at Glaxo will be "Biochemical applications of high resolution chromatography." It is scheduled for 3:00 p.m.

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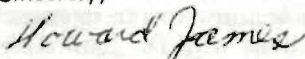
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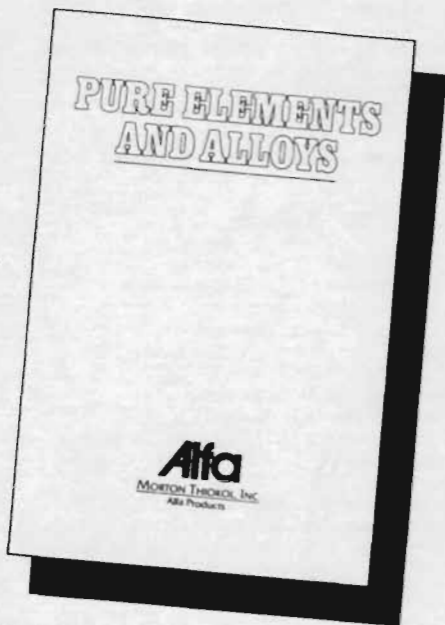
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Changes in membership status also should be submitted to the above address.

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