

THE

TarHelium



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

Vol. 17, No. 2

October 1986

MICROCOMPUTERS IN CHEMISTRY

*A Demonstration of Microcomputer Software
Used in Chemistry*

and

*The Electronic Chemistry Set:
Teaching with Computers*

*A Lecture by
Dr. John W. Moore*

Wednesday, October 22, 1986
Microcomputing Support Center
UNC-Chapel Hill

Software Demonstrations
3:00 — 5:00 P.M.
Venable Hall — Room 307

Lecture
5:30 P.M.
Venable Hall — Room 307

The Microcomputing Support Center in Venable Hall at UNC-Chapel Hill is one of several on the campus. The Venable Hall Center contains 35 IBM PCs, 5 Zenith 148s, 10 Apple IIEs and 10 Macintosh Pluses. Twenty-five of the IBM PCs have 512K of memory and 23 have color monitors. Each of the Zeniths has 512K of memory and a color monitor. The Apple IIEs have 64K of memory and are equipped with monochrome monitors, and the Macintoshes each have external 800K drives.

John W. Moore — Dr. Moore received an A.B. magna cum laude from Franklin and Marshall College and a Ph.D. from Northwestern University, concentrating in physical inorganic chemistry. During 1964-65 he held an NSF postdoctoral fellowship at the University of Copenhagen. He has taught at Indiana University-Bloomington (1965-71), at Eastern Michigan University (1971-present), and during 1981-82 was Visiting Professor at the University of Wisconsin-Madison. He has won several awards for his teaching, including the Catalyst Award of the Chemical Manufacturers Association (1982) and the Michigan Association of Governing Board's Distinguished Faculty Member Award (1982). From 1979 to 1984 he served on the Michigan Environmental Review Board, which advises the Governor of Michigan on environmental quality issues. He has more than 20 years of experience using computers in chemical education and is the author of numerous publications in inorganic chemistry, chemical education, computer applications in chemistry, and environmental chemistry. These include *Environmental Chemistry*, Academic Press, 1976 (with Elizabeth A. Moore), *Chemistry*, McGraw-Hill, 1978 (with W. G. Davies and R. W. Collins), and *Kinetics and Mechanism*, third edition, Wiley-Interscience, 1981 (with Ralph G. Pearson). He is currently editor of the Computer Series feature of the *Journal of Chemical Education* and director of NSF-sponsored Project SERAPHIM, which disseminates micro-computer-based instructional materials. He is active in the ACS Division of Chemical Education, serving as its Program Chair from 1980-82 and as Secretary/Councilor from 1984-86. He is a member of Phi Beta Kappa, Sigma Xi, AAAS, ACS, NSTA, and Phi Kappa Phi.

The Electronic Chemistry Set: Teaching with Computers

The advent of microcomputers that have good graphics capabilities, are easily programmed, are not intimidating to inexperienced student users, and can be obtained at costs similar to or lower than costs of terminals for time-sharing systems will certainly result in major changes in the teaching of chemistry. Computers and the many forms of computer-aided instruction are now available at costs that can be borne by any college or university chemistry department. Moreover, table-top computers are being purchased in large numbers by elementary and secondary schools, and many entering college students are more computer literate than most of their college chemistry teachers. Based on experience in using computers in chemical education, as well as the experience of many others who have reported on their work in the Computer Series feature of the *Journal of Chemical Education*, Dr. Moore will report on the current status of computer applications in chemical education and try to give some inkling of what the future may hold.

VOTE FOR 1987 OFFICERS

North Carolina Section American Chemical Society

Please select one candidate for each office by marking the ballot below.
Mail the ballot, in the enclosed envelope, to:

Dr. John Myers
Department of Chemistry
P.O. Box 19673
North Carolina Central University
Durham, North Carolina 27707

BALLOT VALIDATION IS REQUIRED; to validate your ballot, sign and print your name on the outside of the mailing envelope on the appropriate lines. Election officials must be able to verify your membership before your ballot can be counted.

Brief biographies, provided by the candidates, are included in this issue of *TarHelium*.

OFFICIAL BALLOT

CHAIRMAN-ELECT: ☐ William E. Hatfield
UNC-Chapel Hill

TREASURER: ☐ Joan Bursey
Radian
☐ Reginald Shiflett
Meredith College

COUNCILOR: ☐ Ivy Caroll
RTI
☐ William Little
UNC-Chapel Hill

ALTERNATE COUNCILOR: ☐ William Gutknecht
RTI
☐ Robert Izydore
NCCU

CHAIRMAN-ELECT

William E. Hatfield

A Kentucky native, Dr. Hatfield earned B.S. and M.S. degrees from Marshall University and a Ph.D. from the University of Arizona in 1962. He conducted postdoctoral research at the University of Illinois and joined the faculty at UNC-Chapel Hill as an Assistant Professor in 1963. Dr. Hatfield became a Professor in 1972, a position he continues to hold.

Among his awards are the Arizona-Wilson Fellow, 1961; Continental Oil Fellow, 1961-62; Distinguished Alumnus Award, Marshall University Alumni Association, 1975; Exchange Scientist, National Academy of Sciences, (to Soviet Union), 1977; Guggenheim Fellowship, 1985-86; Charles H. Stone Award, Carolina-Piedmont Section, ACS, 1985; and the Southern Chemist Award, Memphis Section, ACS, 1986.

Dr. Hatfield is a member of the American Chemical Society, the American Association for the Advancement of Science, Sigma Xi, and Materials Research Society of North Carolina.

His professional activities include: Visiting Teacher, North Carolina College, 1964-65; Member, Inorganic Examination Committee, ACS Examinations Committee, 1965-72; Chairman, 1974-1982; Member, Examinations Committee, 1977-1986; Member, Editorial Board, Examinations Institute, ACS, 1986-present; Alternate Councilor, Inorganic Division, 1975-77, 1978-80; Chairman, Awards Committee, NC Section ACS, 1979-81; External Examiner, University of Sierra Leone, Fourah Bay College, Freetown, S. L., Njala University College, Njala, S. L., 1976-78; Consultant, Overseas Liaison Committee, American Council on Education, 1976-78; American Specialist, U.S. State Department, 1977; Director, NATO Advanced Research Institute on Molecular Metals, Les Arcs, France, 1978; Visiting Scholar, Cambridge University, 1978; Member, ACS Awards Committee, 1980-83; Visiting Professor, University of Petroleum and Minerals, Dhahran, Saudi Arabia, 1980; Member, Academic Advisory Council, GTE, Inc., 1980-81; Waite Philip Fishel Lecture, Vanderbilt University, 1981; Visiting Professor, Tata Institute for Fundamental Research, Bombay, India 1981; Guest Professor, Johannes Gutenberg-Universität, Mainz, West Germany, 1982; Visiting Lecturer, University of Puerto Rico, Mayaguez, Puerto Rico, 1982; Member, N.C. Section ACS Awards Committee, 1983-1984; Member, Assessors Panel, The Queen Elizabeth II Fellowships and Australian Research Grants, Committee 1984; Member, Grants Committee, North Carolina Board of Science and Technology, 1984; Treasurer, NC Section, ACS, 1985-1986; Member, Executive Committee, NC Section, ACS, 1985-1986; Member, Awards Committee, ACS, 1986-1989.

TREASURER

Reginald B. Shiflett

Reginald B. Shiflett received his B.S. degree in chemical engineering from the University of Virginia in 1965. He then worked for the DuPont Company as a process engineer and was involved in the pilot plant development of Nomex, the first fiber formed from a wholly aromatic polymer. In 1970 he received his Ph.D. degree in physical chemistry from the University of Virginia and began teaching at Campbellsville College in Kentucky. Dr. Shiflett came to Meredith College in 1978, where he is currently Professor of Chemistry and Department Head. He joined the local ACS section in 1978 and has served on the education and membership committees.

Joan T. Bursey

After receiving a B.S. in chemistry at Creighton University, Joan T. Bursey earned her Ph.D. in chemistry at the University of California-Berkeley in 1969. This circumstance provided her with a somewhat unusual collector's item — a Ph.D. diploma signed by Ronald Reagan, who was governor of California at the time. Upon completion of the Ph.D., Joan Bursey accepted a post-doctoral fellowship at the University of North Carolina-Chapel Hill. Her research advisor at UNC, Dr. Maurice Bursey, felt obligated to locate permanent employment for a post-doctoral fellow and went to rather extraordinary lengths in this case. Marrying one's post-doc will provide permanent employment, but it is a solution to the problem of finding a job for post-docs which can't be used too often. Since both of the Drs. Bursey are mass spectroscopists, there is quite a lot of shop talk in the Bursey household. Joan Bursey worked at the Research Triangle Institute as a mass spectroscopist for fourteen years and has been a Senior Scientist with Radian Corporation for nearly two years. She has taught short courses for the local section of the ACS and served on the nominating committee for several years.

COUNCILOR

Ivy Carroll

Ivy Carroll received his B.S. degree in chemistry from Auburn University in 1957 and his Ph.D. degree from the University of North Carolina, Chapel Hill, in 1961. He joined Research Triangle Institute (RTI) in RTP in 1964 and has been Director of the Organic and Medicinal Chemistry Division of the Chemistry and Life Sciences Unit since 1975. Dr. Carroll's research at RTI has been concerned mainly with the application of organic chemistry to biological problems. Much of his research has involved the synthesis of compounds of potential chemotherapeutic value. He served two consecutive terms on the ACS Offices and Awards Committee from 1980 to 1981 and is presently a member of the Long Range Planning Committee of the Medicinal Chemistry Division of the ACS.

COUNCILOR NOMINEES (cont.)

William F. Little

Bill Little received his Ph.D. degree at UNC in 1954 and did post-doctoral research with Sir Christopher Ingold at University College, London during 1954-55. His first teaching appointment was at Reed College (1955-56) before joining the chemistry faculty in Chapel Hill. His research areas have ranged from early work with ferrocene to organometallic chemistry of transition metals including Co, Ni, Ti, Pt, Ir, and Pd. He was chairman of the department from 1965 to 1970 and Vice Chancellor for (Research), Development and Public Service from 1973 to 1978. He was one of the early "faculty traveling salesmen" who promoted the Research Triangle concept to the chemical industry in the late 1950s and early 1960s.

Dr. Little was on the Governor's Science Advisory Committee, 1961-64, and served on the Executive Committee of the NC Board of Science and Technology for 15 years. He has been chairman of the NC Section of the ACS (1964-65), chairman of the SERM Steering Committee, 1965, and was General Chairman of the 1984 SERM in Raleigh. He served three years on the Steering Committee of the International Conference for Organometallic Chemistry.

Currently Dr. Little is University Distinguished Professor of Chemistry at UNC, a member of the RTI Board of Governors since 1965, and President of the Triangle Universities Center for Advanced Studies, Inc. since 1982.

He was a graduate Morehead Scholar and received the Thomas Jefferson Faculty Award at UNC. He was given the Outstanding Alumnus Award and an honorary DSc Degree from his undergraduate alma mater, Lenoir Rhyne College.

ALTERNATE COUNCILOR

Robert A. Izydore

Dr. Robert A. Izydore received his B.S. degree from Pennsylvania State University and his Ph.D. degree in organic chemistry from Duquesne University. He was an instructor at the McKeesport Campus of the Pennsylvania State University and held a postdoctoral appointment at Duke University before joining the faculty at North Carolina Central University where he is now Professor. Dr. Izydore was chairman of the North Carolina section in 1985 and Treasurer in 1980-81. He has served on the Budget and Nominations Committees and is currently on the Membership Committee.

ALTERNATE COUNCILOR NOMINEES (cont.)

William F. Gutknecht

William F. Gutknecht received his B.S. degree in chemistry from the University of Wisconsin in 1964 and his Ph.D. degree in analytical chemistry from Purdue University in 1970. After post-doctoral work at Louisiana State University, he joined the Chemistry Department of Duke University. Affiliated with the Research Triangle Institute since 1978, he is now manager of the Environmental Chemistry Department. Dr. Gutknecht has been active in the N.C. Section of the ACS for over 15 years. He was chairman of the section in 1981, served on the program, hospitality, membership and nominations committees, and is the incumbent Alternate Councilor. Dr. Gutknecht was editor of *TarHelium* for four years, having just retired from that position.

CALL FOR PAPERS

*1987 EPA/APCA Symposium on
Measurement of Toxic and Related Air Pollutants
May 3-6, 1987*

The next annual national Symposium on Measurement of Toxic and Related Air Pollutants will be held May 3-6, 1987 in the Sheraton Imperial Hotel, Research Triangle Park, North Carolina. The meeting is again cosponsored by the U.S. Environmental Protection Agency's Environmental Monitoring Systems Laboratory and The Air Pollution Control Association.

The technical program will include both invited and contributed papers emphasizing emerging technology in the measurement of toxic and related air pollutants (gases and particulates).

Topic categories include the following: acidic deposition, quality assurance, indoor air pollution, hazardous waste emissions, complex chemical data analysis, source measurements, ambient measurements, wood stove emissions, atmospheric chemistry and measurement application of physico-chemical properties of toxics.

Persons interested in presenting a paper should send a two hundred word proposal abstract, (title, author(s), affiliation(s), and description) by December 15, 1986, to either of the technical program cochairmen listed below. Completed manuscripts (six pages maximum) of accepted papers must be ready by March 31, 1987.

Seymour Hochheiser
Environmental Monitoring
Systems Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711
(919) 541-2106

Dr. R. K. M. Jayanty
Research Triangle Institute
P.O. Box 12194
Research Triangle Park, NC 27709
(919) 541-6483

THE NORTH CAROLINA SECTION, AMERICAN CHEMICAL SOCIETY

Presents Its 1986 Fall Short Course

STATISTICS WITHOUT FEAR

Lecture Dates:

Wednesdays, November 5, 12, 19 and December 3, 10, 1986

Time:

4:30 — 6:30 p.m.

Place:

Auditorium, Main (South) Building,
Burroughs Wellcome Co.,
3030 Cornwallis Road,
Research Triangle Park, NC 27709

Instructors:

Hale Sweeny, Ph.D.,
Burroughs Wellcome Co.

Gerald Hajian, Ph.D.,
Burroughs Wellcome Co.

Dr. Hale Sweeny is head of the Statistical Services Department in the Research and Development Unit at Burroughs Wellcome Co., Research Triangle Park, North Carolina. He has a B.M.E. from Clemson University, an M.S. in industrial engineering and a Ph.D. in mathematical statistics from Virginia Polytechnic Institute. This multidisciplinary background has proved invaluable in teaching numerous applied statistics courses in the pharmaceutical field.

Dr. Gerald Hajian is a Senior Statistician working with Dr. Sweeny at Burroughs Wellcome. He holds a B.S.E.E. from Newark College of Engineering, an M.S. in statistics from Rutgers University, and a Ph.D. in mathematical statistics from Columbia University. For the past 10 years Dr. Hajian has been involved in the design and analysis of preclinical experiments.

COURSE DESCRIPTION:

"Statistics Without Fear" is designed for individuals who need to understand and use statistics but have little or no statistical training. The course is organized around four major themes: introduction to statistical inference; testing of hypotheses; design of experiments, and simple linear regressions. Available software packages will also be discussed. Throughout, the emphasis is on practical applications. A hand calculator will be necessary for homework problems. Solutions to assigned problems will be discussed in detail.

Enrollment is limited to allow time for class discussions. Registrants desiring credit for 1.0 Continuing Education Units (CEU) should check the appropriate line on the registration form below, and add \$5.00 to the fee. For any additional information, call Dr. Monica Nees, Research Triangle Institute, (919) 541-5997.

REGISTRATION FORM

Registration closes October 29, 1986

Enclosed is a check (payable to the NC Section, American Chemical Society) as registration fee for "Statistics Without Fear," the section's short course to be held at Burroughs Wellcome Co., Nov. 5, 12, 19 and Dec. 3, 10, 1986. My cancelled check is my receipt.

- ☐ No charge to unemployed ACS members
- ☐ \$25 high school teachers; full-time students; post-doctoral fellows; retired ACS members
- ☐ \$50 other ACS members
- ☐ \$75 non-members
- ☐ 1.0 CEU desired (add \$5.00)

Name: _____

Phone: _____ Highest Degree: _____

Business Address: _____

Send to: Dr. William Hatfield
Treasurer, NC Section, ACS,
Department of Chemistry 045-A
University of North Carolina at Chapel Hill
Chapel Hill, NC 27514

FUTURE PROGRAMS

Speaker: Clifton E. Melone **Date:** Nov. 19, 1986

Program: "Criminalistics — The Application of Chemistry to Apprehending Criminals"

Location: NCCU

Speaker: NC Distinguished Speaker

Date: Dec. 9, 1986

Location: Meredith College

ADVERTISE IN *TarHelium*

If you market products that are used by chemists, consider advertising in *TarHelium*, the official publication of the North Carolina section of the American Chemical Society.

For more information about *TarHelium* advertisements, contact Dr. Jeff Wilson at (919)248-3433 or write him in care of Burroughs Wellcome Co., Research Triangle Park, NC 27709.

ORGANIC & INORGANIC ANALYSIS

- Chromatography
 - Microscopy
 - Spectroscopy
 - Thermal Analysis
 - Wet Chemical Analysis

For more information, please call or write:

ANALYTICAL SERVICES
Rexham
Industrial

P.O. Box 1377
Matthews, NC 28106-1377
(704) 847-9171

1 9 8 6

FINNIGAN MAT

S E M I N A R

S E R I E S

Seminar 3

Setting New Standards in Magnetic-Sector Mass Spectrometry — The MAT 90

Chapel Hill, NC
Hotel Europa

One Europa Drive

October 31, 1986

Registration/Continental Breakfast

8:30 a.m. to 9:00 a.m.

Program

9:00 a.m. to 12:30 p.m.

Ernst Weber, Ph.D.

Vice President and General Manager, Bremen Operations

Reinhold Pesch, Ph.D.

Research and Engineering Manager, Organic MS, Bremen

Gerd Dielmann, Ph.D.

Product Manager, Magnetic Organic Products, San Jose

Complimentary Lunch

12:30 p.m.

To register, please call Erna Straw (301) 948-1067



Headquarters:
355 River Oaks Parkway
San Jose, CA 95134
(408) 433-4800, USA.
Subsidiaries in FRG, UK,
France, Italy and Japan.

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.

Hannah Green, *Editor*
Allen Jones, *Co-Editor*
Jeff Wilson, *Advertising Manager*

Please direct correspondence to the attention of the editor:

Hannah Green
Burroughs Wellcome Co.
3030 Cornwallis Road
Research Triangle Park, NC 27709

PRE-SORTED
FIRST CLASS MAIL
U.S. POSTAGE PAID
RALEIGH, NC

PERMIT NO. 491

If you wish to change your *TarHelium* mailing address, please submit your old address, your new address and a recent C&EN or *TarHelium* address label to:

Manager, Membership and Subscription Services
American Chemical Society
P.O. Box 3337
Columbus, Ohio 43210

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

Executive Committee:

Eric Bigham, BW, Chairman
William Switzer, NCSU, Chairman-Elect
Carolyn Foust, RTI, Secretary
William Hatfield, UNC, Treasurer
Hannah Green, BW, *TarHelium* Editor
Ivy Carroll, RTI, Councilor
Maurice Bursey, UNC, Councilor
Marcus Hobbs, Duke, Councilor
William Gutknecht, RTI, Alternate Councilor
Halbert Carmichael, NCSU, Alternate Councilor
Henry Bent, NCSU, Alternate Councilor
Louis Quin, Duke, Past Chairman
Bernard Spielvogel, ARO, Past Chairman
Robert Izydore, NCCU, Past Chairman

FIRST CLASS MAIL

0137835L 09/86 ZM 426 1
DR ROBERT GEORGE GHIRARDELLI
US ARMY RES OFFICE
POB 12211
RES TRIANGLE PARK NC 27709