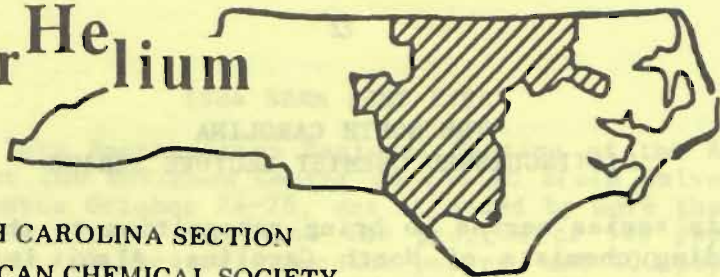


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NORTH CAROLINA SECTION
AMERICAN CHEMICAL SOCIETY

Vol. 15, No. 4

December, 1984

The North Carolina
Distinguished Chemist Lecture Series

Presents

WHAT QUANTUM CHEMISTRY HAS TO SAY ABOUT
THE OLD-FASHIONED CONCEPTS OF CHEMISTRY

by

Dr. Robert G. Parr
William R. Kenan, Jr., Professor
of Theoretical Chemistry
University of North Carolina at Chapel Hill

Tuesday, December 11, 1984

- Social: 5:30 pm, 1887 Room
NCSU Faculty Club
- Dinner: 6:45 pm, President's Dining Room,
Belk Hall, Meredith College
(Members--\$7 Students--\$4)
(See map on Page 3)
- Lecture: 8:00 pm, Carswell Auditorium
Wainwright Music Building
Meredith College

For reservations, please call one of the following by
December 6: In Durham, Sue Dickerson at 684-2414; in
Chapel Hill, Debbie Edwards at 962-2172; and in Ral-
eigh, Joyce Dunn at 737-2548.

THE NORTH CAROLINA
DISTINGUISHED CHEMIST LECTURE SERIES

This series serves to bring recognition to the outstanding chemists of North Carolina. Also, it gives our members the opportunity to hear about the current research being conducted by our distinguished colleagues. This academic year we plan to recognize two speakers. We are pleased to announce that our first distinguished speaker is Professor Robert G. Parr, who will give his presentation at the December meeting at Meredith College.

ROBERT G. PARR, born in 1921, was educated at Brown University and the University of Minnesota. He came to the University of North Carolina in 1974 after serving on the faculties of Carnegie Institute of Technology and Johns Hopkins University. He is a former chairman of the Hopkins Department of Chemistry, of the Division of Chemical Physics of the American Physical Society, and of the Division of Physical Chemistry of the American Chemical Society.

WHAT QUANTUM CHEMISTRY HAS TO SAY ABOUT
THE OLD-FASHIONED CONCEPTS OF CHEMISTRY

Abstract

The contemporary development of computational quantum mechanics into a practical tool for accurately determining molecular properties leaves a major problem: What happens to the simple concepts of structural chemistry and chemical dynamics which have served chemistry so well? Do they disappear or are they preserved? Using ideas from density functional theory, it will be shown that the concepts are in large part preserved, indeed strengthened and made more precise. Special attention will be given to electronegativity, hardness and softness, and the frontier theory of reaction rates.

1984 SERM BEST EVER

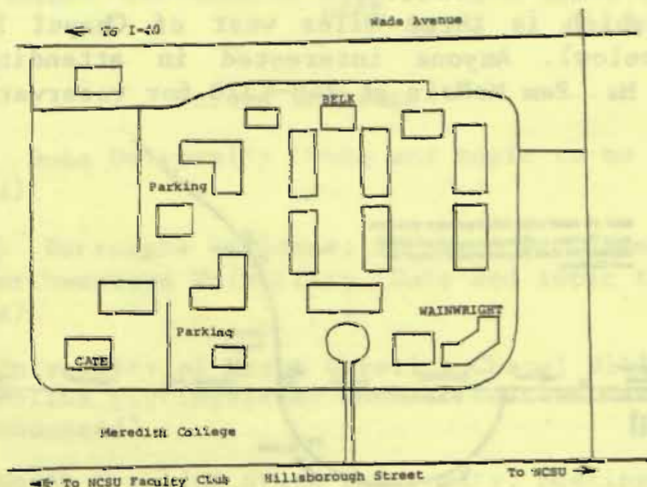
The 36th Southeastern Regional Meeting of the ACS, held at the McKimmon Center on the NC State University campus October 24-26, was attended by more than 1200 registered chemists. The program of 500 papers included 100 invited symposium papers, and 400 papers contributed to general sessions. Special programs included a short course on chemical toxicology, held the day before the meeting; a day-long program for high school teachers, attended by approximately 75 persons; and a special program on microcomputers, to which authors brought and demonstrated original computer programs on laboratory applications and chemical education.

The chemical exposition included 62 exhibitors, the largest number participating in any previous SERM.

At a luncheon on the last day of the meeting, the 1984 Southeastern Region High School Teacher Award was presented to Helen M. Stone of Ben L. Smith High School in Greensboro.

The principal social event, attended by 900 persons, was a mixer featuring hors d'oeuvres with beer and wine, while the Raleigh Little German Band created an Oktoberfest theme.

Generally considered one of the best in recent years, the meeting was a success scientifically and financially and was a credit to its host, our North Carolina Section.



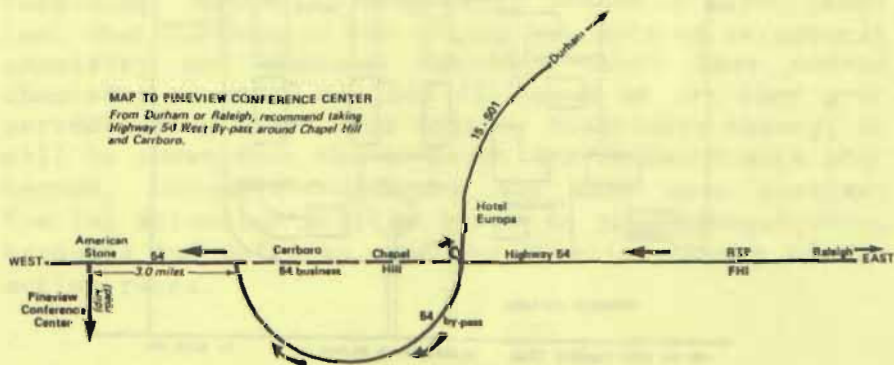
!ALL SECTION MEMBERS WELCOME TO ATTEND!

Planning Retreat at Pineview Conference Center

A second invitation is extended to all interested members of the North Carolina Section to attend a planning retreat on January 26, 1984. The purpose of the retreat is to develop direction and set goals for the Section. The meeting format will include "brainstorming," discussion, prioritization and recommendation of action. A variety of topics will be presented, possibly including the purpose of the Section, promotion of scholarships, awards, education, symposia, content of monthly meetings and new programs. The meeting agenda is to be as follows:

8:00- 8:30	Check-in
8:30- 9:00	Opening Session
9:00-10:30	Period I, Team Discussions
10:30-10:45	Break
10:45-12:00	Discussion of Period I
12:00- 1:00	Lunch (Provided by the Section)
1:00- 2:30	Period II
2:30- 2:45	Break
2:45- 4:00	Discussion of Period II
4:00- 5:00	R & R/Cocktails

This event will be held at Pineview Conference Center, which is three miles west of Chapel Hill (See map below). Anyone interested in attending should phone Ms. Pam McNair at 248-4320 for reservations.



ANNOUNCEMENTS

Dennis G. Wujek Also to Speak at December Meeting

Mr. Dennis G. Wujek, a Duke University graduate student and winner of the 1984 Centennial Scholarship, will present a report on the research supported by the scholarship at the December meeting. The topic area is in the use of lipid bilayers as hosts for organic reactions.

Election Results

The 1984 election results are in and are presented below. Congratulations to the winners. It is unfortunate that not all could win, for each nominee, according to the nominations committee, has served the section extremely well.

Chairman-elect	ERIC BIGHAM Burroughs-Wellcome
Treasurer	WILLIAM HATFIELD UNC-Chapel Hill
Councilor	MAURICE BURSEY UNC-Chapel Hill
Alternate Councilor	HALBERT CARMICHAEL NCSU

Future Meetings

January: Duke University (Date and topic to be announced)

February: Burroughs Wellcome; Speaker: Dr. James A. Ibers, Northwestern University (Date and topic to be announced)

March: University of North Carolina-Chapel Hill, North Carolina Distinguished Chemist Lecture Series (to be announced)

April: North Carolina State University, Meeting in Miniature



CALL FOR PAPERS

**Fifth Annual National Symposium
on
*Recent Advances in
The Measurement of Air Pollutants***

- Topics:** New developments in measuring methods and monitoring systems applicable to:
- Wet and dry deposition
 - Indoor air monitoring
 - Source measurements
 - Personal monitoring
 - Exposure assessment
 - Toxic organics
 - Particles
 - Chemometrics

Sponsor: EPA's Environmental Monitoring Systems Laboratory, Research Triangle Park, North Carolina

Date and Place: May 14 through 16, 1985
Radisson Plaza Raleigh
Raleigh, North Carolina

One-page abstracts should be submitted by January 11, 1985 to Seymour Hochheiser, MD 75, EPA Environmental Monitoring Systems Laboratory, Research Triangle Park, North Carolina 27711.

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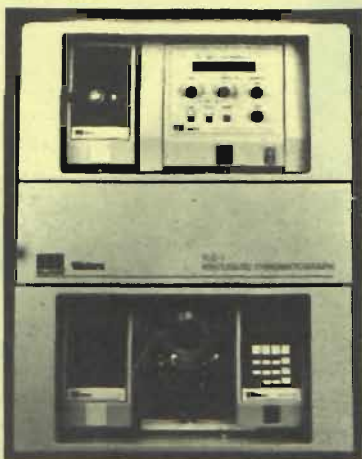
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