



THE

# CHESAPEAKE CHEMIST

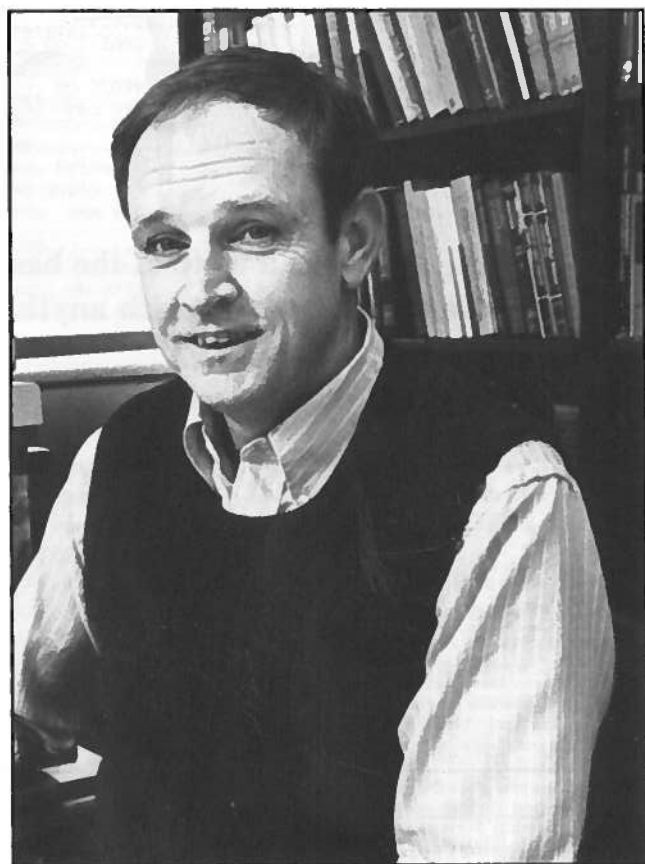
MARYLAND SECTION  
AMERICAN CHEMICAL SOCIETY

VOL. LIII

MAY, 1997

NUMBER 5

## 1997 REMSEN AWARD



**WILLIAM HUGHES MILLER**



# THE CHESAPEAKE CHEMIST

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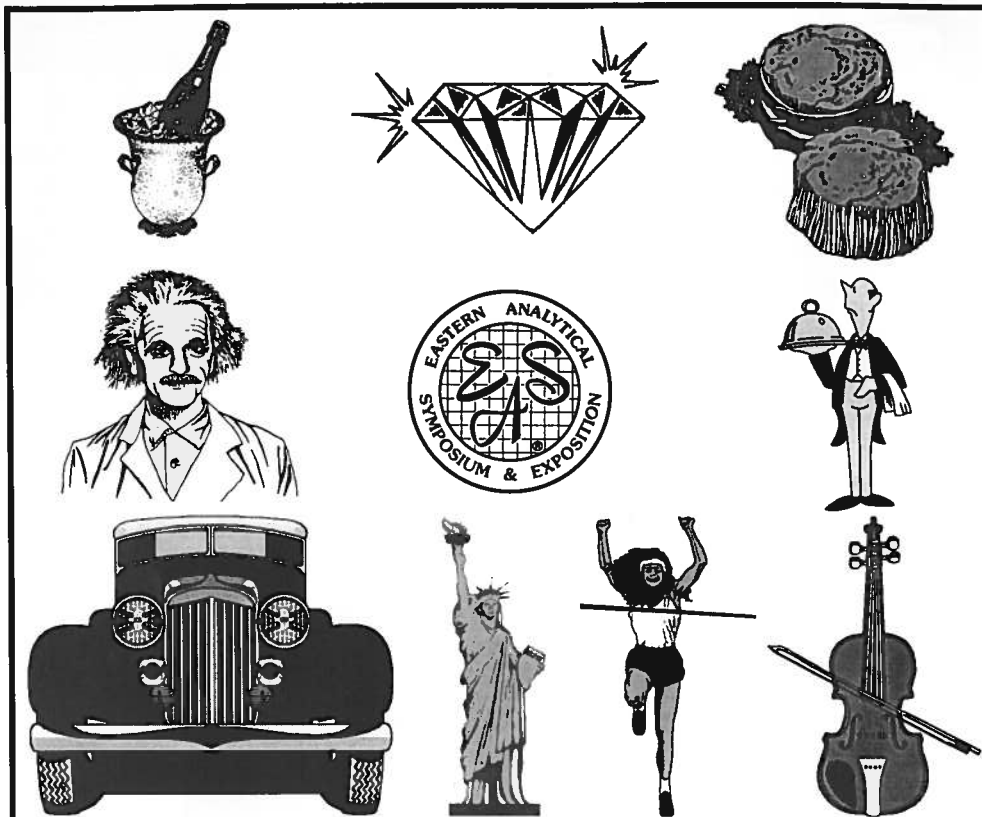
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The 1997 EAS will be held November 16 - 21, 1997 at the Garden State Convention Center and the DoubleTree Hotel in Somerset, New Jersey. You can be part of the 1997 EAS. If you have attended EAS in the past, you are aware of the wide range of papers which are presented at EAS. If you have never attended EAS, but work in the general area of analytical chemistry and the allied sciences, we welcome you to come aboard. You will be surprised to see how many of your colleagues already attend EAS every year. While the general call for papers closed on April 15th, we may still have room for poster presentations in some sessions, and welcome papers in all areas of the analytical and allied sciences. Contact us as soon as possible to see if we can accommodate your paper.

**EAS FACTS IN BRIEF:** EAS is a non-profit [501(c)(3)] scientific organization run totally by volunteer scientists. EAS is proudly sponsored by the Analytical Division and the North Jersey and New York Sections of the American Chemical Society; the American Microchemical Society; the Chromatography Forum of the Delaware Valley; the New York Microscopical Society; and the Delaware Valley, New England, and New York Sections of the Society for Applied Spectroscopy. The 1996 EAS attracted over 5100 attendees and included over 640 Technical Papers, 14 CONFERENCES-IN-MINIATURE, 23 EAS Short Courses, 24 EAS Exhibitor Workshops, 9 Seminars, 9 Tutorials, and 318 exhibit booths. In 1997, the advance Registration fee will remain at a low \$65.

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# THE 52nd REMSEN AWARDEE

The annual Remsen Memorial Lectures were inaugurated in May, 1946 by the Maryland Section of the ACS to honor Ira Remsen, first Professor of Chemistry and second President of the Johns Hopkins University. The Remsen Memorial Lectures are chemists of outstanding achievement, in keeping with Ira Remsen's long and devoted career as an exponent of the highest standards in teaching and research in chemistry.

## WILLIAM HUGHES MILLER

William H. Miller was born in Kosciusko, Mississippi, in 1941, and grew up in Jackson. He received a B.S. in Chemistry from Georgia Tech (1963) and a Ph.D. in Chemical Physics from Harvard (1967). During 1967-69 he was a Junior Fellow in Harvard's Society of Fellows, the first year of which was spent as a NATO postdoctoral fellow at the Physikalisches Institute of Freiburg University (Germany). He joined the chemistry department of the University of California, Berkeley, in 1969 and has been Professor since 1974, serving as Department Chairman from 1989 to 1993.

Professor Miller has made a variety of contributions to the theory of chemical reaction dynamics, molecular scattering theory, and related topics. A comprehensive semiclassical scattering theory showed the physical origin of quantum effects in inelastic and reactive scattering, e.g., interference, tunneling, and 'rainbows' in product state distributions. The first example of 'chaotic scattering' was seen and analyzed within the framework of this S-matrix theory. His formulation of quantum mechanical reactive scattering theory for chemical reactions has been widely used, and more recently the S-matrix version of the Kohn variational principle has been developed into a useful method for carrying out such calculations. A rigorous quantum expression for the rate constant of a chemical reaction was derived which is the intellectual descendent of Wigner and Eyring's transition state theory (an inherently classical theory), and its semiclassical evaluation led to the discovery of the 'instanton', a periodic orbit in imaginary time whose properties determine the reaction rate. The quantum reaction rate was also expressed in terms of a reactive flux correlation function which provides the basis for accurate quantum calculations of reaction rates. Other contributions have been the reaction path Hamiltonian for modeling reaction dynamics in polyatomic molecules, quantum and semiclassical theory of Penning ionization, a method for finding transition states on multidimensional potential energy surfaces, a unified statistical theory for reaction rates, and a combined random matrix/transition state theory for the probability distribution of state-specific unimolecular decay rates.

Professor Miller is a member of the National Academy of Sciences and the American Academy of Arts and Sciences. His awards include the Annual Prize of the International Academy of Quantum Molecular Science (1974), E.O. Lawrence Memorial Award in Chemistry (1985), the Irving Langmuir Award in Chemical Physics (1990), the American Chemical Society Award in Theoretical Chemistry (1994), and the Hirschfelder Prize in Theoretical Chemistry (1996), along with numerous fellowships and invited lectureships.

### BEYOND TRANSITION STATE THEORY - A RIGOROUS QUANTUM THEORY OF CHEMICAL REACTION RATES

Transition state theory (TST) is the ubiquitous model used to characterize the rates of chemical reactions. TST is an inherently approximate model, however, and has no unambiguous quantized form. This lecture describes a rigorous quantum theory of chemical reaction rates, shows its application to a number of simple chemical reactions, and shows how vestiges of TST appear in appropriate cases.

# THE 52nd REMSEN AWARD

## DATE:

Wednesday, June 4, 1997

## PLACE:

Remsen Hall, Room 101  
Homewood Campus  
The Johns Hopkins University

## SPEAKER AND TOPIC:

8:00 pm  
THE REMSEN MEMORIAL LECTURE  
William Hughes Miller  
U. of California, Berkeley  
"Beyond Transition State Theory  
- A Rigorous Quantum Theory of  
Chemical Reaction Rates."

Dinner price is \$17.00 per person,  
but spouses and retired chemists  
may attend for \$15.00; students  
may attend for \$9.00.

## DINNER:

The Johns Hopkins University  
Shriver Hall  
Clipper Room  
Reception 6:00 pm  
Dinner 7:00 pm

Dinner reservations should be made  
by mailing checks, payable to  
Maryland Section of ACS, to

Dr. Shirish Shah  
College of Notre Dame  
4701 North Charles Street  
Baltimore, MD 21210

by May 28. Late reservations may  
be made by calling

(410) 532-5712

by May 30. An answering machine  
is available at this number.

It is not necessary to be a member of the American Chemical Society to attend. You may attend the lecture without attending the dinner.

## PREVIOUS REMSEN AWARD WINNERS

|      |                         |      |                       |
|------|-------------------------|------|-----------------------|
| 1996 | David Evans             | 1970 | George S. Hammond     |
| 1995 | Alfred G. Redfield      | 1969 | Albert L. Lehninger   |
| 1994 | Edward I. Solomon       | 1968 | Har G. Khorana        |
| 1993 | Christopher T. Walsh    | 1967 | Marshall W. Nirenberg |
| 1992 | William Klemperer       | 1966 | Paul H. Emmett        |
| 1991 | Rudolph A. Marcus       | 1965 | James R. Arnold       |
| 1990 | Robert G. Bergman       | 1964 | Paul D. Bartlett      |
| 1989 | K. Barry Sharpless      | 1963 | Harold C. Urey        |
| 1988 | Mildred Cohn            | 1962 | George Porter         |
| 1987 | Stephen L. Lippard      | 1961 | Herbert C. Brown      |
| 1986 | Gilbert Stork           | 1960 | Henry Eyring          |
| 1985 | Richard N. Zare         | 1959 | Edward Teller         |
| 1984 | Earl L. Muetterties     | 1958 | Robert B. Woodward    |
| 1983 | George M. Whitesides    | 1957 | Melvin Calvin         |
| 1982 | Harden McConnell        | 1956 | Farrington Daniels    |
| 1981 | Koji Nakanishi          | 1955 | Willard F. Libby      |
| 1980 | Roald Hoffmann          | 1954 | Vincent du Vigneaud   |
| 1979 | Harry B. Gray           | 1953 | Edward L. Tatum       |
| 1978 | John Charles Polanyi    | 1952 | W. Mansfield Clark    |
| 1977 | Ronald Breslow          | 1951 | Hugh S. Taylor        |
| 1976 | William N. Lipsomb, Jr. | 1950 | Edward C. Kendall     |
| 1975 | Henry Taube             | 1949 | Joel H. Hildebrand    |
| 1974 | Elias J. Corey          | 1948 | Elmer V. McCollom     |
| 1973 | Frank H. Westheimer     | 1947 | Samuel C. Lind        |
| 1972 | Charles H. Townes       | 1946 | Roger Adams           |
| 1971 | George C. Pimentel      |      |                       |

#### UPDATE FROM THE CHAIR

Hi! I'd like to present an overview of Maryland Section activities since my letter last July.

#### Recent accomplishments:

- \* Acceptance of our award as outstanding local section (medium-large category) by Shekar Munavalli and our councilors.
- \* Internet workshop, spectroscopy workshops, visit to EPA lab in Annapolis. (Mike Zapf)
- \* Outstanding student awards. (Carl Minnier)
- \* Gateway to Chemistry program at UMBC - 150 participants. (Lawrence Boucher)
- \* Science fairs at Morgan and Towson. (Mike Zapf, Elwin Penski, others)
- \* Chemical Bonding Day and Demo days. (Frank Millio)
- \* Maryland Chemist Award to Shekar Munavalli.
- \* Kids and Chemistry program - 2,000 students from Baltimore City, Baltimore County, Anne Arundel County, Montgomery County, Howard County, Harford County and Maryland Science Center. (Mark Greenberg, Anna and Bella Kraut, Victoria Kuntz, Shirish Shah, Alfred Amah, Angela Sherman, Shekar Munavalli, Ernie Silversmith, science teachers, parents, college and high school students and support from others, including ACS.)

#### Future activities planned or in progress:

- \* Remsen Award on June 4th. (Bill White and Mike Zapf)
- \* Retired chemists lunch on May 23rd. (Elwin Penski, Alvin Bober, Shirish Shah)
- \* Fall dinner meetings. (Jan Kolakowski, Mike Zapf)
- \* National Chemistry Week. (Victoria Kuntz, Mark Greenberg)
- \* Kids and Chemistry. (Shirish Shah, Anna Kraut, Victoria Kuntz, Sue Kastfanos)
- \* Possible participation in Maryland Science Teachers annual meeting. (Mark Greenberg, Frank Millio, Shirish Shah, Victoria Kuntz)
- \* Possible high school teacher award. (Kathleen Thompson)
- \* Selection of chair and program chair for MARM.
- \* Educational workshop day similar to the Gateway to Chemistry, possibly in the spring. (Lawrence Boucher, Mark Greenberg, Shirish Shah)

As you can see, we are active, and we need your help, ideas and suggestions to make us visible in the community. So please communicate with us and let us know how we can better serve your needs. Have a good summer.

Truly,  
*Shirish Shah*

#### SEPTEMBER MEETING

Our September meeting is scheduled for Wednesday, September 17 at College of Notre Dame. Dr. Rita Boggs will discuss job opportunities in chemical industry.

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#### STUDENT AWARDEE

An additional student awardee, too late to make our April issue, is Robin Kloster of Mount Saint Mary's College.

#### SERMACS-97

The Southeastern Regional Meeting will be held October 19-22, 1997 at the Roanoke Airport Marriott and Clarion Hotels.

The deadline for submission of abstracts is June 1. Abstracts, on standard ACS abstract forms, should be sent to Dr. Tomas Hudlicky, Program Chair, Department of Chemistry, University of Florida, Gainesville, FL 32611. Telephone (352) 392-9844.

#### NOMINATING COMMITTEE REPORT

Chair Shekar Munavalli of the nominating committee reports the following slate of officers and councilors for 1988:

Chair Jan Kolakowski                      Secretary Anna Kraut  
Vice Chair Mark Greenberg              Treasurer Robert von Tersch  
Chair-elect Kathleen Thompson

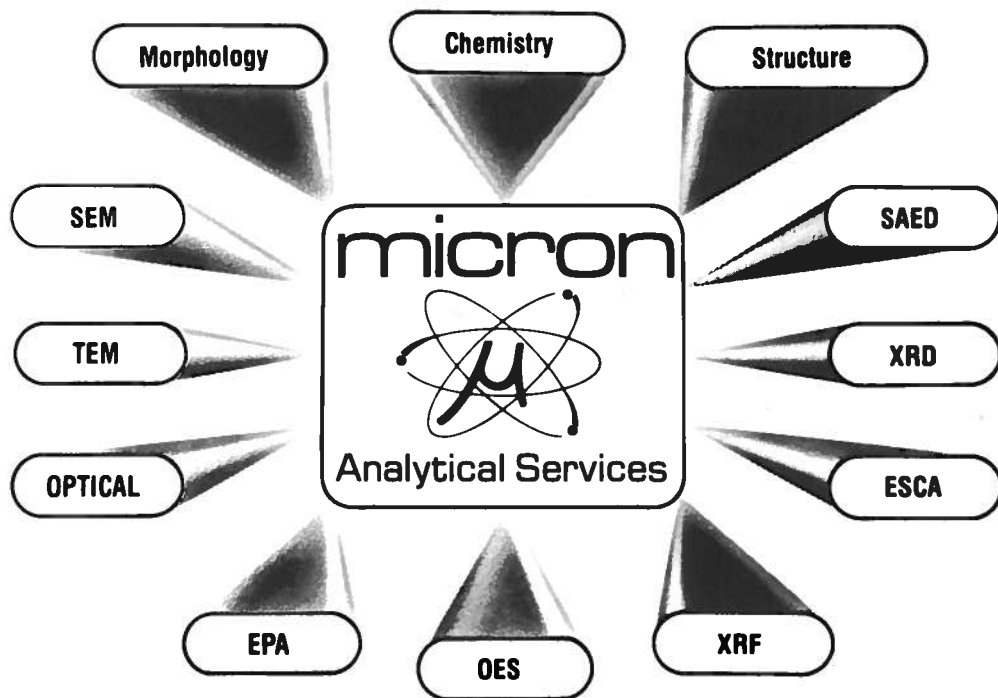
Alternate Councilors Shekar Munavalli  
Joseph Topping  
Linda Sweeting

Members-at-large Donald Hoster              Catherine Fenselau  
Dale L. Whalen                              Asoka Katumuluwa  
Mike Ellzy

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#### SCIENCE FAIRS

Mike Zapf expresses his and our thanks to the many members who helped in judging the Morgan State Science and Engineering Fair and the Baltimore Science Fair at Towson State University on March 22nd.

Judges included Elwin Penski, Mark Gold, Joseph DeVance, Maggi Wilcox, Charles Tumosa, Asoka Katumuluwa, Mike Ridge, Roger Collins and Tom Brewer.

Maryland Section presented major awards consisting of a plaque and a United States Savings Bond as well as certificates of merit in both middle school and high school categories at each fair.

Major awards at Morgan went to Evan Rabinowitz of Woodlawn High School and Kimberly McDowell of Sudbrook Middle School. At Towson senior awards went to Timothy Winters of Atholton High School and Elizabeth Gladmon of Woodlawn High School, while the middle school award went to Derek Potter of St. Anthony.