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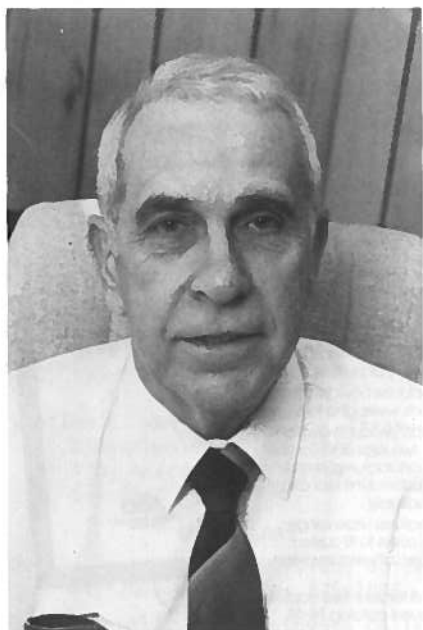
CHESAPEAKE CHEMIST

MARYLAND SECTION
AMERICAN CHEMICAL SOCIETY

VOL. XLIII

FEBRUARY, 1987

NUMBER 2



FREDERICK W. LAMPE



JOYCE J. KAUFMAN

Colloquia are held at 4:15 pm in Remsen Hall room 221 on the Homewood Campus of The Johns Hopkins University. Refreshments are served before each colloquium at 4:00 pm. For more information contact Mrs. H.J. Potter, 338-7421.

DATE	SPEAKER AND AFFILIATION	TITLE
February 3	Millard H. Alexander University of Maryland	Collisional Electronic Energy Transfer in Diatomic Molecules
February 10	Gary Brudvig Yale University	To be announced
February 17	Paul Wender Stanford University	To be announced
February 24	Josef Michl Univ. of Texas at Austin	To be announced
March 3	To be announced	
March 10	Terry A. Miller Ohio State University	To be announced
March 17	James M. Lisy University of Illinois	Vibrational Predissociation Spectroscopy of Molecular Clusters

THE 21ST MARM

The 21st Middle Atlantic Regional Meeting will be held May 19-21 at Stockton State College, Pomona, NJ.

The meeting will feature about 20 symposia as well as general papers in most areas of chemistry.

The General Chairman is Dr. Shelby Broughton, Stockton State College, Pomona, NJ 08240

PITTSBURGH CONFERENCE

The Pittsburgh Conference and Exposition on Analytical Chemistry and Applied Spectroscopy is scheduled on March 9-13. Future meetings are in line for New Orleans, Atlanta, New York and Chicago.


Advance registration for 1987 costs \$35 with lower rates for students and spouses and rate increases for on-site registration.

Registration Chairman is Dr. John Novak, 12 Federal Drive, Pittsburgh, PA 15235.

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Joyce Kaufman received her B.S., MA. and Ph.D. degrees in Chemistry from The Johns Hopkins University and a D.E.S. Trés Honorable in Theoretical Physics from the Sorbonne, Paris, France. She then joined the staff at the Research Institute for Advanced Studies (RIAS), where she was Head of the Quantum Chemistry Group from 1962 to 1969. In 1969 she returned to Johns Hopkins as Principal Research Scientist in the Department of Chemistry at the University and Associate Professor in the Department of Anesthesiology in the School of Medicine.

She is the recipient of the Garvan Medal of the American Chemical Society and the Maryland Chemist Award. She is on the editorial boards of a number of scientific journals. Dr. Kaufman is active in the American Chemical Society and is the Senior Councilor for the Division of Physical Chemistry and serves on the ACS Committee on Budget and Finance. She is also a past Chairman and a past Councilor of the Maryland Section.

Her research interests are in the application of theoretical chemistry to fields ranging from energetic compounds to biomedical molecules.

AB-INITIO QUANTUM CHEMICAL CALCULATIONS ON LARGE MOLECULAR SYSTEMS AND CRYSTALS

Ab-initio quantum chemical calculations on a variety of systems investigated have made it possible to predict correctly molecular properties and reactivities prior to experiment. These calculations have been carried out with methods derived in her group incorporating a number of desirable computational strategies which make much more tractable such computations on large molecules.

The examples to be discussed include energetic compounds, the mechanism of cationic polymerization and biomedical molecules. Also some recent results on ab-initio potential functions for intermolecular interactions will be mentioned. Such potentials are important in predicting crystal densities, transport properties, biomolecular interactions and other phenomena.

FREDERICK W. LAMPE

Frederick W. Lampe was born in Chicago, Illinois on January 5, 1927. His primary and secondary education was received in the public schools of Amityville, New York and was completed in 1944. From 1944-46 he served in the U.S. Navy and upon being discharged from the service in 1946 he began his higher education at Hunter College. He received the B.S. degree from Michigan State University in 1950 and the A.M. and Ph.D. degrees from Columbia University 1951 and 1953, respectively. He was married to Eleanor F. Coffin on March 26, 1949 and they have five children.

From 1953-1960 he was engaged in research in physical chemistry with the Humble Oil and Refining Company in Baytown, Texas. In 1960, he accepted an appointment as Associate Professor of Chemistry at The Pennsylvania State University, becoming Professor of Chemistry in 1965 and Head of the Department of Chemistry in 1983. In 1966-67 he was a National Science Foundation Senior Postdoctoral Fellow and Visiting Professor at the Physics Institute of the University of Freiburg in West Germany. During 1973-74 he was a United States Senior Scientist Awardee of the Alexander von Humboldt Foundation of West Germany and Visiting Professor at the Hahn-Meitner Institute for Nuclear Research in West Berlin. He returned to the Hahn-Meitner Institute as a Senior Scientist Awardee of the von Humboldt

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FEBRUARY MEETING

DATE:

Wednesday, February 18, 1987

PLACE:

Knott Science Center
The College of Notre Dame of
Maryland
North Charles Street
Baltimore

SPEAKERS AND TOPICS:

5:30 pm
Frederick W. Lampe
Pennsylvania State Univ.
'The Infra-red Laser Photo-
chemistry of Silanes'

8:00 pm
Joyce J. Kaufman
The Johns Hopkins Univ.
'Ab-initio Quantum Chemical
Calculations on Large Mole-
cular Systems and Crystals'

COCKTAILS AND DINNER:

Doyle Building Dining Room
Social Hour 6:30 pm
Dinner 7:00 pm

Dinner price \$12.00 per person, but spouses, retired chemists and students may attend for \$10.00

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

John Corliss
P.O. Box 20899
Baltimore, MD 21209

by February 9. Late reservations may be made by calling

John Corliss at (301) 235-6612 or Nolan Phillips at (301) 939-3500

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

1986-1987 MARYLAND SECTION PROGRAM

DATE AND LOCATION	SPEAKER	AFFILIATION
March 11, 1987 College of Notre Dame	John Lever Glen Prestwich	The Johns Hopkins Univ. SUNY at Stonybrook
April 22, 1987 Hood College	Student Awards Plus 3 under 30 Bober, Riley and Cohen Science Fair Winners' Posters	
May, 1987	Rensen Award	

DIVISION OF PROFESSIONAL RELATIONS

We have been asked by Raquel Diaz-Sprague, chair of the Professional Relations Committee of the Columbus Section, to aid in soliciting new members for the ACS Division of Professional Relations. The DPR works for expansion of the employment rights of chemical professionals and, of course, its representation on the ACS Council depends on the size of its membership.

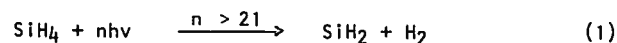
Annual dues of the Division are \$4.00 and membership can be arranged through Paul A. Rebers, Secretary, Division of Professional Relations, P.O. Box 70, Ames, Iowa 50010.

...cont. from p 4

Foundation and Visiting Professor in the Summer of 1984. He is a member of the American Chemical Society and a Fellow of the American Physical Society. His principal research interests are in the area of ion-molecule reactions and gaseous free-radical reactions in photochemistry and radiation chemistry. A list of publications during the last five years is attached.

THE INFRARED LASER PHOTOCHEMISTRY OF SILANES

Silane is decomposed readily by the absorption of infrared radiation from a CO₂ TEA laser, the P(20) line of the 10.6 m band being a particularly convenient frequency. The molecule does not, however, decompose in the collision-free region; collisions involving V-V transfer are necessary for a molecule to accumulate sufficient energy to dissociate. This primary dissociation in the collision-assisted photodecomposition of SiH₄ is that of the lowest energy decomposition and may be written.



Dissociation to SiH₃ + H, the next higher energy process, requires 30-40 kcal./mol more energy (11-15 more infrared photons) and is not observed to any significant extent. This formation of SiH₂, without the simultaneous formation of SiH₃, is unique to the infrared photochemistry of SiH₄ and provides, therefore, a useful method to study the reactions of SiH₂.

In neat SiH₄, the insertion reactions of SiH₂ result in the formation of the observed final products: H₂, Si₂H₆, Si₃H₈, Si₄H₁₀, Si₅H₁₂ and a solid containing silicon and hydrogen. At a fluence of 1.0J/cm², the results are accounted for, quantitatively, by the assumption of a Boltzmann distribution of vibrational quanta in the SiH₄ molecule during the pulse and a reaction mechanism similar to that thought to obtain in the thermal decomposition of SiH₄.

SiH₄ is also decomposed readily by energy transfer from SiF₄ molecules which have undergone infrared multiphoton excitation from the 1025 cm⁻¹ line from a CO₂ TEA laser. In contrast to the irradiation of pure SiH₄, the only products observed are H₂ and Si₂H₆. The absence of higher silanes is attributed to the fact that reactant SiH₄ molecules are less vibrationally excited in the sensitized process than in the decomposition of neat SiH₄.

Both types of laser-induced decomposition provide a means to study the reactions of SiH₂ free from complications caused by the presence of SiH₃. Studies of the reactions of SiH₂ with HCl, CH₃Cl, PH₃, GeH₄, D₂ and NO will be discussed.

ACS DEPARTMENT OF GOVERNMENT RELATIONS AND SCIENCE POLICY HAS TAKEN INITIATIVES IN BIOTECHNOLOGY

Biotechnology is emerging as a prominent field for our nation's scientific research and development initiatives. During 1986, the ACS Department of Government Relations and Science Policy (GRASP) has become involved in biotechnology, which uses chemistry as a major component for its development.

Early this year GRASP published an information pamphlet entitled "Biotechnology." This primer, written for the nonscientist, explains the scientific basis of biotechnology, defines what is meant by biotechnology, what it can and cannot do, and where the science could lead. "Biotechnology" also examines public concerns about the environmental release of genetically engineered organisms.

In May, GRASP and the National Bureau of Standards coordinated and sponsored a Conference on "The Chemical Aspects of Biotechnology," which was cosponsored by 22 ACS Divisions, related organizations, and federal agencies. The conference encompassed both the technical and policy aspects of biotechnology. Participants examined the technical developments in the field as well as the controversial policy issues, such as whether current law is adequate to regulate biotechnology products, how major chemical companies are accommodating this evolving industry, and how new biotechnology firms are faring.

GRASP also has been involved in other biotechnology initiatives. This past spring, GRASP staff arranged for members of the ACS Task Force on TSCA (Toxic Substances Control Act) to conduct technical briefings for congressional staff. These congressional staff are trying to determine whether greater federal regulation of the biotechnology industry is necessary at this time and are working on legislative proposals to coordinate federal activities relative to biotechnology.

A bill was introduced in the Senate, S.1967, "the Biosafety Act," amending the Toxic Substances Control Act (TSCA) to protect the environment and human health from adverse effects, which may be caused by the release of genetically-engineered micro-organisms into the environment. S.1967 was referred to the Senate Environment Committee's Toxic Substances and Environmental Oversight Subcommittee, which did not conduct hearings on the legislation during the 99th Congress. Another bill, the "Biotechnology Science Coordination Act of 1986," (H.R.4452) was introduced in the House, which would amend TSCA to control genetically engineered organisms. This bill would also establish a committee within the Office of Science and Technology Policy to coordinate federal activities involving the science of biotechnology. H.R.4452 was referred to three House committees--Science and Technology, Energy and Commerce, and Agriculture. The House Science and Technology's Subcommittees on Agriculture Research and the Environment and on Science, Research and Technology, held hearings on June 4 and 5, 1986. ACS testified before these Subcommittees (ACS Statement 86-022) on June 5.

In late summer, GRASP staff organized an informal network for Washington-based organizations that have a professional and organizational interest in the developing field of biotechnology and its related public policy implications. The "Biotech Network" members will meet regularly to exchange information, which is of mutual interest, about activities in the area of biotechnology.

The GRASP Department hopes that its involvement in several biotechnology projects throughout this past year will serve as the initial step in developing and maintaining a policy and monitoring base for ACS activities in this growing field. During the next session of Congress, it is likely that the legislative proposals to monitor and regulate biotechnology that surfaced during the 1985-86 congressional session will be reintroduced. GRASP will continue to follow the progress of biotechnology initiatives on Capitol Hill as well as in the executive branch and agencies of the federal government.

Michele M. Boisse

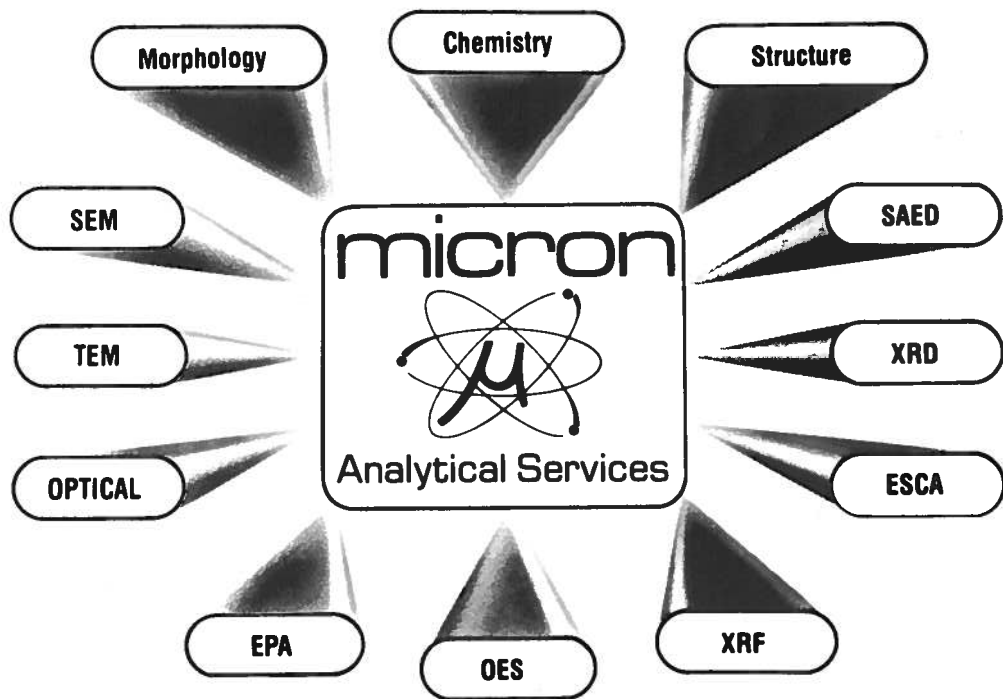
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