



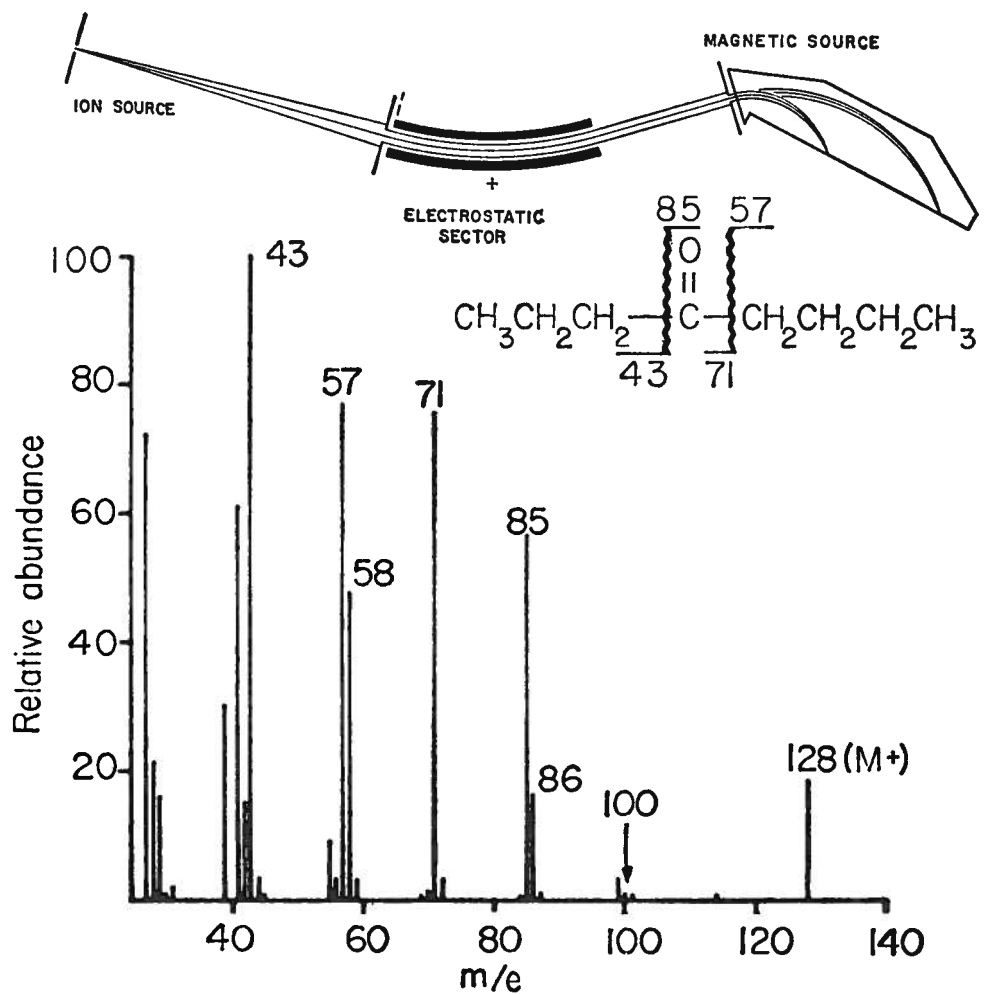
# THE CHESAPEAKE CHEMIST

MARYLAND SECTION  
AMERICAN CHEMICAL SOCIETY

VOL. XXX

SEPTEMBER, 1974

NUMBER 6



# EXECUTIVE COMMITTEE MINUTES

Minutes of the Executive Committee Meeting of the Maryland Section of the American Chemical Society held on May 22, 1974 at McCormick & Co., Inc., Hunt Valley, Maryland.

Present: A. Bednarczyk, Y. Caplan, J. Cogliano, H. Cohen, R. Ellin, F. Gornick, D. Jones, J. Kolbe, M. Miller, R. Schneider, T. Simmons, K. Zeller.

The meeting was called to order by the Chairman, D. Jones at 8:15 p.m. The minutes of the meeting of January 30, 1974 were approved as reported in the March issue of the Chesapeake Chemist.

The treasurer's report as prepared by E. Silversmith was presented by M. Miller. The cash balance on hand as of May 15, 1974 was \$11,244.29.

In the absence of the Award Committee Chairman, D. Jones presented the report of that Committee. The Committee is seeking nominations for the regional award for high school teachers and nominations for the E. Emmet Reid Award for outstanding teaching at a small college.

M. Miller reported on the activities of the Education Committee. The recently conducted short course on Ion Selective Membrane Electrodes drew 46 participants and was operated at a net cost of \$15 to the Section. Future plans of the Committee were discussed and it was anticipated that more extensive courses will be offered in the future.

D. Jones explained the reason why the press release about the Remsen Award made no mention of the Maryland Section and indicated that the oversight will not occur in the future. He also indicated that the Remsen Award Committee is seeking nominations for next year's award.

It was suggested that the Scholarship Committee be disbanded since its work has now been completed. In the absence of the Committee Chairman, however, this motion was tabled.

A. Bednarczyk presented the program for next Fall and Spring. This program will be published in the Chesapeake Chemist in the Fall.

K. Zeller of the Chesapeake Chemist requested \$1500 to settle accumulated bills for the publication costs of the Chesapeake Chemist. The request was approved.

H. Cohen reported on his search for a new printer for the Chesapeake Chemist. His choice was approved and it is expected that the next issue of the Chesapeake Chemist will be printed by the new printer.

A lengthy discussion ensued on the costs of dinner meetings. Some Executive Committee members favored an increase of \$1.00, others an increase of \$0.50. In light of the expected decrease in the cost of producing the Chesapeake Chemist with the new printer, the Committee agreed to the \$0.50 increase. Accordingly, dinner costs next Fall will be \$5.50 for members and \$3.50 for students.

Some discussion followed in regard to changing the honorarium associated with the Remsen Award. The secretary was directed to obtain information from the National Office about honoraria associated with other local section awards.

The meeting was adjourned at 10:25 p.m.

Respectfully submitted,  
Melvin P. Miller  
Secretary

## Nominations for New Officers

The nominating committee is seeking suggestions for future officers of the Section. Contact any of the following with your suggestions.

Dr. Joyce Kaufman, Chairman  
The Johns Hopkins University  
366-3300 Ext. 1359

Dr. Yale Caplan  
State Medical Examiners Officer  
396-3845

Dr. Tom Simmons  
Edgewood Arsenal - 671-4148

Dr. Jim Leslie  
Univ. of Md., Baltimore - 528-6573

Dr. Herb Aaron  
Edgewood Arsenal - 671-2156



# THE CHESAPEAKE CHEMIST

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Ernest F. Silversmith.....Treasurer  
Chemistry Department  
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Baltimore, Maryland 21212

## COMMITTEE CHAIRMEN

Awards and National  
Nominations..... William Galetto  
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Chemical Education..Melvin Miller  
323-1010

House and Program... A. Bednarczyk  
667-7480

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531-5711

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Publicity..... Dave Roswell  
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323-1010

Remsen Award..... Brown Murr  
366-3300

Scholarship..... E. Silversmith  
323-2270

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COVER: (top) Schematic diagram of a high resolution mass spectrometer (bottom) Mass spectrum of octan-4-one. (Courtesy F.W. McL.)

The Chesapeake Chemist is published monthly September through May by the Maryland Section of the American Chemical Society. Address editorial comments to Howard J. Cohen, Glidden-Durkee, Div. of SCM Corp., 3901 Hawkins Point Road, Baltimore, Md. 21226. Phone 633-6400. Address advertising inquiries and copy to Kent R. Zeller, McCormick & Co., Inc., 204 Wight Ave., Hunt Valley, Md. 21031.

## MARYLAND CHEMIST AWARD

The Maryland Chemist Award was established in 1962 to recognize and honor each year, a member of the Maryland Section for outstanding achievement in the field of chemistry. The achievement may be in pure or applied chemistry, chemistry, chemical engineering or chemical education. The award is presented annually at one of the regular meetings of the Maryland Section.

Recipients to date have included:

1962 Dr. E. Emmet Reid	1968 Dr. George L. Braude
1963 Dr. W. Mansfield Clark	1969 Dr. Leslie Hellerman
1964 Dr. Alsoph H. Corwin	1970 Dr. Paul H. Emmett
1965 Dr. John C. Krantz, Jr.	1971 Dr. Giles B. Cooke
1966 Dr. Belle O. Talbot	1972 Dr. Arnold M. Seligman
1967 Dr. Walter S. Koski	1973 Dr. Lester P. Kuhn

The nominee must be a member of the American Chemical Society and a member of the Maryland Section. The meritorious achievement of the nominee shall have been accomplished within the five years previous to that in which the award is given. A previous recipient of the award is not eligible for re-nomination. If in a particular year there is no nominee deemed by the Award Committee to meet the qualifications required, the award shall not be made.

Nominations may be submitted in any format but must include, in addition to the name and present position of the nominee, your specific reasons as to why this Section Member should be so honored.

Nominations should be submitted to any of the undersigned not later than September 20, 1974.

Dr. David W. Herlocker  
Member, Awards Committee  
Department of Chemistry  
Western Maryland College  
Westminster, Md. 21157

Dr. Gary Posner  
Member, Awards Committee  
Department of Chemistry  
The Johns Hopkins Univ.  
Baltimore, Md. 21218

Dr. William G. Galetto  
Chairman, Awards Committee  
McCormick & Co., Inc.  
204 Wight Avenue  
Hunt Valley, Md. 21031

### -----Tear Out Dinner Reservation Form -----

There is enclosed \$ \_\_\_\_\_ (\$5.50 per person)\* for dinner reservations at Eudowood Caterers, Eudowood Plaza, for the following persons.\*\*

<u>Name</u>	(Please print or type)	<u>Affiliation</u>
-------------	------------------------	--------------------

\*Please make checks payable to Maryland Section, ACS and mail together with reservation form to Dr. Allen Bednarczyk, McCormick and Co., Inc., 204 Wight Avenue, Hunt Valley, Md. 21031, or phone 667-7470, 667-7480.

\*\* Return by Friday preceding next meeting.

## SEPTEMBER MEETING

DATE:

WEDNESDAY, SEPTEMBER 18, 1974

PLACE:

Eudowood Gardens Lecture Room,  
Eudowood Plaza, Joppa Road near  
Goucher Boulevard.

SPEAKERS AND TOPICS:

5:30 PM  
Dr. Klaus Biemann, MIT  
"Applications of a Gas Chroma-  
tograph-Mass Spectrometer-  
Computer System"

8:30 PM  
Dr. Fred McLafferty  
Cornell University  
"Developments in Organic Mass  
Spectrometry"

SOCIAL HOUR:

There will be a social hour after  
the meeting. Refreshments will  
be served.



DR. FRED McLAFFERTY



DR. KLAUS BIEMANN

COCKTAILS AND DINNER:

Eudowood Gardens Dining Room  
Cocktails 6:30-7:15 courtesy of  
DuPont Instruments Division.  
Hot buffet dinner (7:15) \$5.50  
per person. Retired chemists,  
students and their spouses may  
attend the dinner at \$3.50 each.  
Reservations are necessary for  
the dinner and should be made  
with

Dr. Allen Bednarczyk  
McCormick and Co., Inc.  
204 Wight Avenue  
Hunt Valley, Maryland 21030  
Phone 667-7480, 667-7470.

It is not necessary to be a  
member of the American Chemical  
Society to attend the dinner or  
the talks, and the talks may be  
attended without attending the  
dinner. You are invited to bring  
your wife and friends to both the  
dinner and the meeting.



## Fred W. McLafferty

Fred W. McLafferty received his B.S. and M.S. from the Univ. of Neb. in 1943 and 1947, respectively. He was in the U.S. Army 1943-1945 serving in Europe in the infantry. He received his Ph.D. degree from Cornell Univ. in 1950, and held a post-doctorate fellowship at the Univ. of Iowa. From 1950-1956 he was in charge of mass spectrometry and gas chromatography in the Spectroscopy Laboratory of the Dow Chemical Co. in Midland, Mich., after which he was Director of Dow's Eastern Research Lab. in Framingham and Wayland, Mass. In 1964 Dr. McLafferty moved to Purdue Univ. as Professor of Chemistry, where he also established and directed the regional Mass Spectrometry Center sponsored by the NIH. In 1968 he became Professor of Chem. at Cornell University.

Dr. McLafferty's chief scientific interests are in analytical chemistry, mass spectrometry for molecular structure determination, and on-line computer techniques. He has been author of "Mass Spectrometry of Organic Ions" (1963), "Mass Spectral Correlations" (1963), "Interpretation of Mass Spectra" (1966 and 1973), "Index and Bibliography of Mass Spectrometry" (with J. Pinzelik, 1967), and "Atlas of Mass Spectral Data" (with Profs. Stenhagen and Abrahamsson, 1969), and co-editor of "Advances in Analytical Chemistry and Instrumentation" (1966-72), and "Archives of Mass Spectral Data". He is a founding member of ASTM E-14, now the American Society for Mass Spectrometry, and he has been Secretary, Committee Chairman, Delegate, and on the Executive Committee. His "Short Course" on mass spectrometry was one of the first offered by the ACS; this course has now been presented more than 20 times to over 1,000 students.

Dr. McLafferty's activities in the ACS include Chairman of the Div. of Analytical Chemistry, Chairman of the Midland Section, and Chairman-elect and National Councilor of the Northeastern Section. He is or has been a member of the following Editorial Advisory Boards: "Analytical Chemistry", "Accounts of Chemical Research", the ACS "Advances in Chemistry" Series, "Organic Mass Spectrometry", "Spectroscopy Letters",

"Applied Spectroscopy Reviews", Handbook of Spectral Data", and the Kolthoff-Elving "Chemical Analysis Series".

Dr. McLafferty was Plenary Lecturer, Anniversary Meeting, the Chemical Society, Glasgow, 1965; Sigma Xi-RESA National Lecturer, 1966; Stauffer Lecturer, UCLA, 1966; Franklin Lecturer, Univ. of Kansas, 1967; Career Scholars Lecturer, Univ. of Nebraska, 1968; Visiting Professor, Univ. of Washington, 1968 and Univ. of Western Ontario, 1969; American Cyanamid Lectureship, Univ. of Connecticut, 1969; Plenary Lecturer, International Mass Spectrometry Meeting, Kyoto, 1969; Distinguished Visiting Professor, Univ. of Iowa, 1969; Plenary Lecturer, International Mass Spectrometry Meeting, Brussels, 1970 the A.D. Little Lecturer, Northeastern Univ., 1971, and F. C. Phillips Lecturer, Univ. of Pittsburgh, 1972. He received the ACS Award in Chemical Instrumentation for 1971 and a John Simon Guggenheim Fellowship for 1972.

## Developments in Organic Mass Spectroscopy

Despite the wide acceptance of mass spectrometry as a major tool for research and analytical problems in a wide variety of organic and biological systems, recent advances give promise of even greater capabilities in the future. Sensitivity is a unique advantage of mass spectrometry; GC/MS systems with capabilities for identification of nanogram samples and detection of picogram samples are now commercially available. A new system for liquid chromatography/MS will be described which gives on-line monitoring and identification with high sensitivity. A system for "signal enhancement in real-time" greatly increases the speed and sensitivity of data collection in high-resolution mass spectrometry, making possible GC/MS at high resolution and routine operation at much higher resolving powers. This is accomplished by computer directed rescanning of peaks in vacant regions of the mass spectrum. The large volume of data from a mass spectrometer is a problem as well as an advantage; a "probability based matching" system for retrieval of reference spectra and a "self-training interpretive and

retrieval system" for computer interpretation of the spectra will be described. The former requires 10 sec. and the latter 1.5 minutes on a lab size dedicated computer utilizing a reference collection of 30,000 mass spectra. Collisional activation spectra provide a new technique for the characterization of the structures of ions. This appears to have broad applications for elucidation of the mass spectra of more complex molecules by defining the structures of the fragments shown in their mass spectra.

## Klaus Biemann

Klaus Biemann was born in Innsbruck, Austria on November 2, 1926. In 1951, he received his Ph.D. from the University of Innsbruck. From 1951 to 1955, Dr. Biemann was an Instructor at the Univ. of Innsbruck. In 1955, he came to MIT as a Research Associate and has progressed through the positions of Instructor, Assistant Professor, Associate Professor and in 1963 was promoted to his present position of Professor of Chemistry.

Dr. Biemann is an Honorary Member of the Belgian Chemical Society and the recipient of the Stas medal in gold from the Belgian Chemical Soc. (1962). Dr. Biemann was the recipient of the Tricentennial Medal of the Univ. of Innsbruck (1970). He is a Fellow of the American Academy of Arts and Sciences and received a Fulbright Fellowship in 1954. He has lectured extensively in the U.S. and foreign countries including Plenary Lectures, UPAC-Symposia on Natural Products, Brussels 1962, Kyoto 1964, and other international symposia. He was also the Venable Lecturer at the Univ. of North Carolina in 1971. He was a member of the Advisory Board of Analytical Chemistry (1968-1971) and since 1967 has served in a similar capacity for Organic Mass Spectrometry.

Dr. Biemann has published over 140 papers in the fields of natural products structure and synthesis, development of mass spectrometric techniques and their application to the determination of the structure of natural products. Dr. Biemann has also concentrated much effort into the use of computers in high resolution mass spectrometry and the

combination of a gas chromatograph with a mass spectrometer. Dr. Biemann is also the author of "Mass Spectrometry: Organic Chemical Applications"

## GC-MS-Computer System

With the advent of the direct interfacing of a mass spectrometer with a gas chromatograph a few years ago it became possible to very efficiently attack certain problems involving complex mixtures. The most complex and most interesting mixtures are those produced by biological systems and GC-MS has therefore been most conspicuously applied to biochemical and biomedical problems. More advanced systems used a computer for data acquisition and processing because the volume of data generated by an efficient GC-MS system by far exceeds what can be handled and utilized manually with any amount of human patience. The GC-MS-computer system developed at MIT has been in routine use for a few years and was applied to a variety of problems. Foremost among them was the development and use of a technique for the sequencing of protein derived large oligopeptides by their partial degradation by acid hydrolysis or enzymatic cleavage to a mixture of smaller peptides which still contain all the sequence information. Chemical derivatization (conversion to O-TMS polyamino alcohols) makes them amenable to gas chromatographic separation and mass spectrometric identification.

On the other extreme, the GC-MS-computer combination is the central part of an almost fully automated, fast method for the identification of drugs and their metabolites in body fluids. It is used routinely in emergency cases of drug intoxication, mainly in the accidental ingestion by children.

A series of computer techniques have been developed to efficiently use the vast amount of data recorded in a single experiment in which mass spectra are recorded continuously. The resulting information is much more than one would have obtained from individual scans at certain points in the gas chromatogram, or the selective processing of the mass spectral data.

\*\*\*\*\*

L'SHONAH TOVAH TIKOSEVAH

## MARYLAND SECTION MEETINGS 1974 - 1975

Date	Time	Speaker/Subject	Location
Sep. 18, 1974	5:30 P.M.	Dr. Klaus Beimann - MIT GC/MS-COMPUTER SYSTEM	Martin's Eudowood *du Pont Instrument Division
	8:30 P.M.	Dr. Fred McLafferty - Cornell University DEVELOPMENTS IN ORGANIC MASS SPECTROMETRY	
Oct. 16, 1974	5:30 P.M.	Dr. David Hoy - David Hoy Associates - LECTURES AND DEMONSTRATIONS OF EXTRA- SENSORY PERCEPTION (ESP)	Notre Dame College *Beckman Instruments *VWR Scientific
	8:30 P.M.		
Nov. 20, 1974	5:30 P.M.	Dr. Jack Kwiatek - U.S. Industrial Chem. Co. HOMOGENEOUS CATALYTIC HYDROGENATION	Martin's Eudowood *Scientific Products
	8:30 P.M.	Prof. Roald Hoffmann - Cornell University THEORETICAL ASPECTS OF PENTACOORDINATION	
Dec. 18, 1974	8:30 P.M.	MARYLAND CHEMIST AWARD	Notre Dame College *Hewlett-Packard
Jan. 15, 1975	5:30 P.M.	WORLD FOOD CRISIS	Martin's Eudowood
	8:30 P.M.	Dr. Richard L. Hall - McCormick & Co., Inc. FOOD SAFETY	*McCormick & Co., Industrial Flavor Division
Feb. 19, 1975	5:30 P.M.	Dr. James Little - Waters Associates INTRODUCTION TO LIQUID CHROMATOGRAPHY	Martin's Eudowood *Waters Associates *Perkin-Elmer
	8:30 P.M.	Dr. Jack Kirkland - du Pont (Title of talk to be given later.)	
Mar. 19, 1975	5:30 P.M.	ACUPUNCTURE	Martin's Eudowood
	8:30 P.M.	Dr. G Melville Williams - Johns Hopkins Hospital ORGAN TRANSPLANTS/BIOCHEM- ISTRY OF REJECTION	*Fisher Scientific
Apr. 16, 1975	8:30 P.M.	To be announced	U.M.B.C.
May 1975	8:30 P.M.	REMSEN AWARD	Johns Hopkins *Varian Associates *Macalaster Bicknell

\*Cocktail Hour Sponsor

## THE JOHNS HOPKINS UNIVERSITY

Some current news from the Dept. of Chemistry is as follows:

Dr. Peter Y. Johnson has the following lecture: "The Synthesis and Reactions of 6-Alkoxytetrahydro-1, 3-oxazines - A New Class of Antineoplastics," Northern Virginia Community College, 833 Little River Turnpike, Annandale, Virginia, The Chemical Soc of Washington, 809th Meeting, Thurs., May 9th, 1974.

Dr. Masato Koreeda has the following publication: "Invertebrate Endocrinology and Hormonal Heterophyly," K. Nakamshi, M. Koreeda, and D. A. Schooley, ed. by W. J. Burdette, Springer-Verlag, N.Y., 1974, pp. 204-217.

Dr. Richard J. Kokes has the following publications: "Butene Isomerization over Zinc Oxide and Chromia," C. C. Chang, W. C. Conner, and R. J. Kokes, J. Phys. Chem. 77, p. 1957 (1973).

"Characterization of Adsorbed Intermediates on Zinc Oxide by Infrared Spectroscopy," R. J. Kokes, Accounts Chem. Res. 6, p. 226 (1973).

"The Nature of Molecular Hydrogen Adsorbed on Zinc Oxide," C. C. Chang, L. T. Dixon, and R. J. Kokes, J. Phys. Chem. 77, p. 2634 (1973).

"The Nature of Molecular Nitrogen Adsorbed over Zinc Oxide," C. C. Chang and R. J. Kokes, J. Phys. Chem. 77, p. 2640 (1973).

"Intermediates in the Oxidation of Propylene Over Zinc Oxide," B. L. Kugler, and R. J. Kokes, J. Catal. 32, p. 170 (1974)

Dr. Gary H. Posner has been promoted to Associate Professor as of July 1, 1974.

Dr. Emil H. White has the following publication: "Chemically Produced Excited States," Emil H. White, Jeffrey D. Miano, Carol J. Watkins, Eves J. Breau, *Angewandte Chemie* (English Edition), 13, pp. 229-243 (1974); German Ed., 86, pp. 292-307 (1974).

## LOYOLA COLLEGE

Four Loyola faculty members have been named Outstanding Educators of America for 1974, it was announced today.

Francis P. Fairbank, Dr. Henry C. Freimuth, Dr. Lucy C. Kotarides, and Dr. Melvin P. Miller were selected for the honor based on their professional and civic achievements.

Outstanding Educators of America is an annual awards program honoring distinguished men and women for exceptional service and leadership in the field of education.

Chairman and assistant professor emeritus in Loyola's Education Dept., Francis P. Fairbank spent 38 years in the Baltimore City school system before joining Loyola full time in 1967. He is a 1927 alumnus of Loyola College.

Professor of chemistry, Dr. Henry C. Freimuth was a toxicologist in the office of Maryland's Chief Medical Examiner for 28 years before coming to Loyola full time in 1972. A native of New York, he has taught at the University of Maryland Medical School and the Johns Hopkins School of Hygiene.

Dr. Lucy C. Kotarides is associate professor and chairwoman of the College's Special Education Dept. Her specialization is in the area of emotionally disturbed children, and she has numerous professional and civic memberships in this area to her credit, including service in a 1970 White House Conference on Children and Youth.

At the present time, Dr. Melvin P. Miller, professor of chemistry, holds a fellow-by-courtesy designation from Johns Hopkins University where, in 1972, he conducted research through a National Science Foundation grant. A 1957 graduate of Loyola, he is secretary of the Maryland section of the American Chemical Society.

### COPY DEADLINE

Copy for the *Chesapeake Chemist* should be forwarded to the Editor not later than the fifth of the month preceding publication.



## VIEWPOINT

Whether our personal political viewpoint tends to be liberal (Government surely ought to do something to help people), or conservative (Those dunderheads in the legislature are continually interfering in our lives and fouling things up), our reactions to government and politics can run from fascination to frustration, and from incredulity to sheer apathy.

Yet in a sense we get the quality of government we deserve. However, much disdain we have for politicians and politics, the democratic system by its very definition requires broad-based participation to work well. Members of the scientific and technological communities, by virtue of their capacity and training to think clearly and objectively, can make valuable contributions not only to government itself, but also to the process of choosing our elected officials, i.e. to politics.

Apart from lobbying and public education programs our Society may undertake to affect government policy, and apart from the role some take as science advisors to government, there are several ways an individual can take a share in local, county, and state politics. The whole idea here is to help put people you want into office by doing more than just voting. There are two general approaches. One is to volunteer for the campaign staff of your preferred candidate. Or lacking any, encourage someone of your acquaintance, who is active in the community, to consider the possibilities of running for office.

The other approach is through the structures of party politics. Both major parties in Maryland have a state chairman, county chairmen, and local precinct leaders. One way to begin is to contact any of them and volunteer for work in your party's precinct organization. Or inquire at county or state party headquarters. Another route is to join and become active in a political club. Many have local politicians as speakers and members, and the political contacts available at club meetings or hang-outs are invaluable for a gut-level education in political realities.

With a little experience as a political volunteer, either for an individual candidate or the party, you could consider running for election to your party's state central committee, the policy-making and governing body of the party. Since it is the function of a party to recruit, develop, and elect candidates to office, it is at the central committee level where one can begin to influence candidate development on a county or state-wide basis.

Then with sufficient practical experience in campaigning and politics, you might eventually decide to run for county council or the General Assembly yourself. But whether you commit yourself to a little or a lot, your awareness of the political scene through participation will score against the dunderhead politician and in favor of effective government.

David J. Heiser

Editor's Note: Dr. Heiser is a chemist and a member of the Republican Central Committee of Anne Arundal County.

### ORGANIC MICROANALYSES

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## ACS NEWS

ACS Manpower Policy Committee  
Dr. Bernard Friedman, Chairman

Dear Colleagues:

There are encouraging signs that the federal government may begin large scale scientific and technical work on the energy problem which will directly involve many professionals including chemists and chemical engineers.

To me it is obvious that substantially all of the organizations of professionals permitted the establishment of elaborate mission oriented organizations such as the AEC and NASA without adequate consideration of how these operations should be phased out when necessary.

Whether such projects are to be done directly by the government or by contractors, some orderly pre-arranged method needs to be set up to avoid the short term employment shocks which such mass discharges have repeatedly produced.

In the final report of our committee, I believe that we should include that the ACS, as a matter of policy, is opposed to the establishment of large scale mission oriented scientific and technical projects which do not include civil service or similar protections for employees that fully meet employment standards such as our own guidelines for employers and also do not have humane and reasonable methods for termination which prevent dumping of human resources when their release will upset the employment market.

Sincerely yours,

Emerson Venable

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