



THE CHESAPEAKE CHEMIST

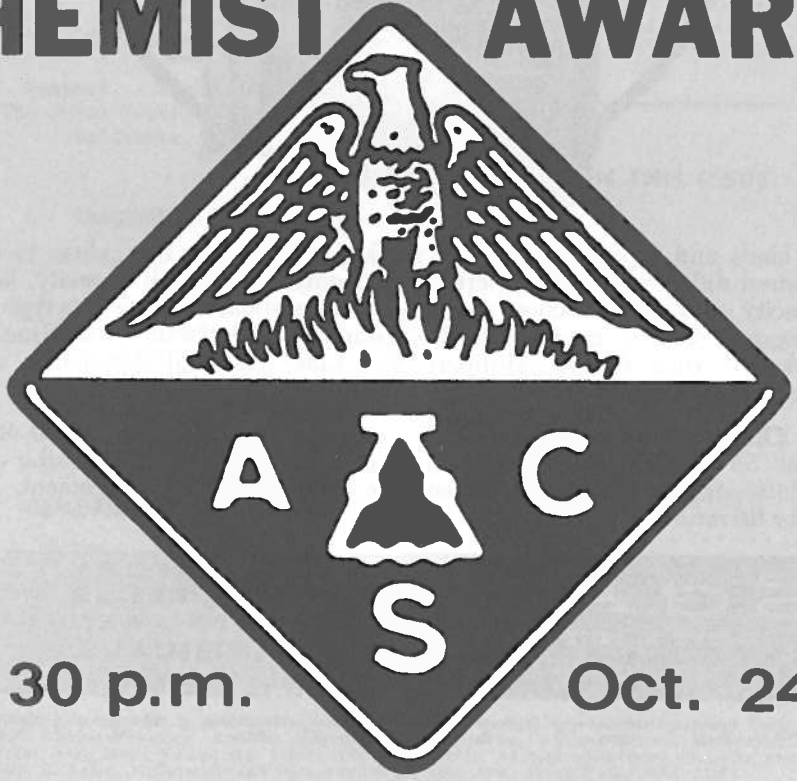
MARYLAND SECTION
AMERICAN CHEMICAL SOCIETY

VOL. XXIX

OCTOBER, 1973

NUMBER 7

MARYLAND CHEMIST AWARD



8:30 p.m.

Oct. 24

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THE CHESAPEAKE CHEMIST

VOL. XXIX

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The Chesapeake Chemist is published monthly September through May by the Maryland Section of the American Chemical Society. Address editorial comments to Dr. William Galetto, McCormick and Co., 204 Wight Ave., Hunt Valley, Md. 21031. Phone 666-3155. Address advertising inquiries and copy to Mr. Kent R. Zeller, McCormick and Company, 204 Wight Ave., Hunt Valley, Md. 21031.

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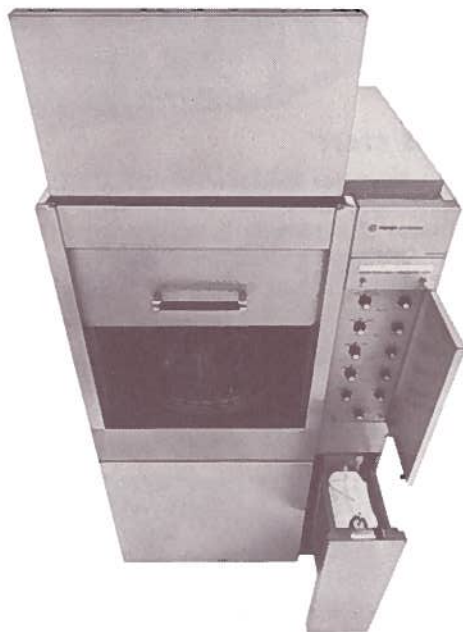
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OCTOBER MEETING

MARYLAND CHEMIST AWARD

DATE AND TIME:

Wednesday, October 24
1973 at 8:30 P.M.

PLACE:

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

SPEAKER:

Dr. Lester P. Kuhn, Chief
Chemist and a Ballistic
Research Fellow, Aber-
deen Proving Grounds.

SUBJECT:

"Hydrogen Bonding of
Organic Mono and Diols"

COCKTAILS AND DINNER:

Eudowood Gardens Dining
Room. A pay bar (0.50 ea)
will be available. Price
is \$5.00 for a hot Buffet
dinner (7:15 P.M.). Stu-
dents and retired chemists
and their spouses may at-
tend the dinner for \$3.00.
Reservations are necessary
for the dinner, and should



Dr. Lester P. Kuhn

be made with Mr. Allen
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Inc., 204 Wight Ave., Hunt
Valley, Md. 21031, phone
667-7470 no later than the
Friday preceding the meet-
ing. It is not necessary
to be a member of the ACS
to attend the dinner or
the talks, and the talk
may be attended without
attending the dinner.
You are invited to bring
your wife and friends to
both the dinner and the
meeting.

SOCIAL HOUR:

There will be a social
hour after the meeting.
Refreshments will be
served. All are wel-
come.

Dr. Lester P. Kuhn

Lester P. Kuhn was born in Brooklyn, New York on July 5, 1913. He received his B.S. degree from Alfred University and his Ph.D. from the Johns Hopkins University in 1948. At the Hopkins he worked under the tutelage of Professor Alphonse Corwin. In 1950-51 Dr. Kuhn was the recipient of a Guggenheim Fellowship and spent the year at Oxford University where he worked with Sir Harold Thompson. In 1958 he was awarded a Secretary of the Army Research Fellowship and spent the year at the Federal Institute of Technology in Zurich, Switzerland.

Dr. Kuhn came to the Interior Ballistic Laboratory in 1942 shortly after the outbreak of World War II and has been there ever since. He is presently Chief Chemist and a Ballistic Research Fellow. In 1965 he received the Robert H. Kent award. Awarded annually since 1957, this award is given to an outstanding scientist or engineer of the BRL.

Dr. Kuhn has been visiting professor at Michigan State University where he gave a series of lectures on infrared spectroscopy from the organic chemist's point of view. In 1968 he received a certificate of outstanding achievement for a paper he presented at the Army Science Conference at West Point. He is also the author of over 60 publications, a number of government reports and 5 patents. His publications cover a wide range of subjects including propellant chemistry, hydrogen bonding, infrared spectroscopy, conformational analysis, kinetics and mechanism of organic and inorganic reactions.

Dr. Kuhn has been a counsellor of the American Chemical Society, a member of its publication committee, the British Chemical Society, the American Society for the Advancement of Science and Sigma Xi.

COPY DEADLINE

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

HYDROGEN BONDING OF ORGANIC MONO AND DIOLS

By measuring the intensities of the free and bonded OH bands one can readily obtain conformational equilibrium constants of cis and trans cyclohexane diols and of cis and trans alkyl substituted cyclohexane diols. The shift in the OH band, $\Delta\nu$, is also easily obtained. It seems to be related to the length of the hydrogen bond A-H...B.

The value of $\Delta\nu$ has been determined for a number of cis and trans cycloalkane-1,2-diols when the number of carbon atoms in the ring varies from 5 to 16. In rings smaller than cyclodecane OH groups are closer together in the cis diol than in the trans diol. In rings larger than cyclodecane the trans diols are closer than the cis.

The bands due to free and internally bonded OH groups have been measured for various substituted ethylene glycols having the structures R_2COHCH_2OH , meso and racemic $(RCHOH)_2$ and $(R_2COH)_2$ where R is methyl, ethyl, isopropyl and t-butyl. In the racemic series of 1,2-disubstituted ethylene glycols, all the compounds exist in the conformation which allows the OH groups to be cis. In the meso series, where R is a normal alkyl group the OH groups are again cis but when R is isopropyl the predominant conformation has the OH groups trans, and when R is t-butyl the conformation is exclusively trans. In each series of compounds increasing the steric requirements of R decreases the distance between the OH groups as indicated by an increase in $\Delta\nu$. Tetra-t-butylethylene glycol with a $\Delta\nu$ of 170 cm^{-1} has the strongest hydrogen bond of any diol thus far reported. It is suggested that the repulsion between the alkyl groups on the adjacent carbon atoms of the substituted glycol produces a deformation of the molecule which allows these groups to be farther apart and at the same time causes the OH groups to be brought closer together. The deformation may be either a decreasing of the O-C-C bond angles or a bending of the central C-C bond.

The equilibrium constant for the equilibrium, nonbonded conformations \rightleftharpoons hydrogen bonded conformations, was determined for 2-methoxyethanol (I),

3-methoxypropanol-1 (II), and 4-methoxybutanol-1 (III) in CCl_4 solution over the temperature range of 0 to 60° , and values of ΔF , ΔH , and ΔS were obtained. Similar data were also obtained for the association between 1-butanol and butyl ether. The half band width, $\nu_{1/2}$, and the change in intensity with temperature, dB/dT , are much larger for the intermolecularly bonded OH band than for the intramolecularly bonded OH band. Although $\Delta\nu$ increases by a factor of 6, there is little change in ΔH , indicating that the Badger-Bauer rule does not hold for intramolecular bonds. Hydrogen bond formation in I is more exothermic than expected because it is accompanied by loss in repulsive nonbonded interactions. Hydrogen bond formation in III is less exothermic than expected because it is accompanied by an increase in repulsive interactions. The Badger-Bauer rule is obeyed by II because in this instance the hydrogen bond interaction is the major contributor to ΔH . The equilibrium constant becomes smaller in going from I to III because ΔS becomes larger. The change in entropy is related to the ratio, number of hydrogen bonded conformations/number of nonbonded conformations.

IF YOU CHANGE YOUR ADDRESS . . . Please do not notify the Editor of the *Chesapeake Chemist*, but send your new and old addresses to: The American Chemical Society, 1155 Sixteenth Street, N. W., Washington, D. C. 20036. The Maryland Section will then be notified.

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EMPLOYMENT OPPORTUNITIES

The Maryland Section of the ACS has learned of the need for a Pharmaceutical Chemist in the State of Md. Dept. of Health and Mental Hygiene, Bureau of Laboratories. The work requires routine identification tests and other analytical studies on pharmaceutical products and requires the applicant to have a minimum B.S. degree and three years' experience in chemistry or an M.S. with at least one year of experience in chemistry. (Ph.D. would be desirable.) Interested applicants should contact Dr. Nathan Levin, Maryland State Bureau of Laboratories, 16 E. 23rd Street, Baltimore, MD 21218, phone 383-2865.

McCormick & Co., Inc. - Laboratory Technician for pesticide residue analyses on spices, poultry, oleoresins, etc. First year college chemistry and pesticide residue experience preferred. Some experience with gas chromatography, either industrial or academic, required. Contact Allen Bednarczyk, McCormick & Co., Inc., 204 Wight Ave., Hunt Valley, Md. 21031 (667-7480, 667-7470).

NOVEMBER MEETING

November 21, 1973



Dr. Frank H. Westheimer (center), Professor at Harvard University, receives the 1973 Remsen Award of the Maryland Section of the ACS from Dr. Yale H. Caplan (right), Chairman of the Section. Dr. Harry Woolf (left), Provost of the Johns Hopkins University, represents the University.

DR. JOYCE J. KAUFMAN WINS 1974 GARVAN MEDAL

Dr. Joyce J. Kaufman of the Johns Hopkins University is 1974 winner of the American Chemical Society's \$2,000 Garvan Medal, given annually to an outstanding woman chemist of the U.S. The announcement was made during the Society's recent week-long national meeting in Chicago.

Dr. Kaufman, who is principal research scientist in the university's chemistry department and associate professor of anesthesiology in its School of Medicine, is being recognized for her exceptional achievements in the services to chemistry.

Internationally acclaimed for her theoretical work, she recently has applied computer calculations to predict the behavior of large drug molecules, such as those in morphine, that affect the central nervous system.

She has given invited lectures on this subject at numerous meetings and institutions both in the U.S. and abroad, including the prestigious Karolinska Institute in Stockholm.

An active member of the American Chemical Society since 1951, Dr. Kaufman currently is representing the Division of Physical Chemistry on the ACS Council. She also has served as chairman and councilor of the society's Maryland section, and as a member of several ACS committees.

The award, which Dr. Kaufman will receive next April during the Society's 167th national meeting in Los Angeles, was established in 1936 through a donation from the noted lawyer and philanthropist Francis P. Garvan "to recognize distinguished service to chemistry by women chemists, citizens of the U.S."

MARYLAND CHEMIST AWARD

This award was instituted in 1962 to recognize and honor meritorious achievement in pure or applied chemistry, chemical engineering, or chemical education, of an outstanding caliber by a member of the Maryland Section.

The award consists of a scroll and is presented annually at one of the regular meetings of the Maryland Section. The reproduction shown on the front cover is that of one of the scrolls presented.

Nominations are solicited from the local membership and an Award Committee appointed by the Section Chairman, may also nominate and will select the recipient.

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 renomination.

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.

Selection is made before the May meeting and presentation is made in the fall of the year.

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 D. Kuhn

ACS Short Courses

Oct. 13-14. Maintaining and Troubleshooting Chromatographic Systems. John Walker, M. Jackson, and M. Bradley. Washington, D.C.

Oct. 13-14. Organic Synthesis—Modern Reactions and Approaches. Dr. Barry Trost and Dr. Edwin Vedejs. Rochester, N.Y.

Oct. 25-27. Polymer Chemistry. Dr. John Stille and Dr. James Mark. Philadelphia, Pa.

Nov. 8-10. Principles of Color Technology. Dr. Fred Billmeyer, Jr. Cleveland, Ohio.

Nov. 17-18. Intermediate Gas Chromatography. Dr. Harold McNair, Dr. Richard Juvet, Jr., and Dr. Stuart Cram. New York City.

Nov. 17-18. Modern Liquid Chromatography. Dr. Lloyd Snyder and Dr. J. Kirkland. New York City.

Nov. 30-Dec. 1. Interpretation of Mass Spectra. Dr. Don DeJongh. New York City.

Dec. 9-14. Minicomputers and Interfacing. Dr. Raymond Dessy and David Larsen. Blacksburg, Va.

When Did YOU

Last Attend An

ACS Meeting?

A BICENTENNIAL COMMEMORATION OF
THE DISCOVERY OF OXYGEN
APRIL 23-26, 1974
TREADWAY INN, WILKES BARRE, PENN.

The Ninth Middle Atlantic Regional Meeting of the American Chemical Society will be held at the Treadway Inn in Wilkes Barre, Pennsylvania, on April 23-26, 1974. On Thursday the meeting will feature a bicentennial commemoration of the 1774 discovery of oxygen by Joseph Priestley. This portion of the program will be a Priestley Symposium; a steam engine railroad trip to the historic Priestley home in Northumberland, Pa.; presentation of the 1974 Priestley Medal at the home; and a commemorative banquet.

Dr. Bennett Willeford, Chemistry Department, Bucknell University, Lewisburg, Pa., is the technical program chairman and is calling for papers in the traditional areas to be given at the meeting. The abstracts of papers deadline is January 1, 1974.

Invited speakers and topics for the Priestley Symposium are: Dr. Ervin Hiebert, Professor of History of Science, Harvard University, "The Integration of Revealed Religion and Scientific Material in the Thought of Joseph Priestley;" Dr. Robert E. Scholfield, Professor of History, Case Western Reserve University, "Priestley as a Scientist;" and Dr. Aaron J. Ihde, Professor of Chemistry, University of Wisconsin, "Priestley and Lavoisier."

The general chairman of the meeting is Dr. James J. Bohning, Chairman of the Chemistry Department, Wilkes College, Wilkes Barre. The host is the Susquehanna Valley Section. The middle Atlantic region of the American Chemical Society consists of the Central Pennsylvania, Delaware, Lehigh Valley, Maryland, Monmouth County, Philadelphia, Princeton, Southeastern Pennsylvania, South Jersey, Susquehanna Valley, Trenton, Washington, and Western Maryland Sections.

1974 ACS CHARTER FLIGHT TO SOUTH AMERICA

For the first time the American Chemical Society (Polymer Division) is organizing for 1974 a Charter Flight to South America! We plan to leave New York by VARIG 707 jet for two weeks on Tuesday, July 23, 1974, pick up southern and western participants by stopping at Miami, and then proceed directly to Brasilia, newly-created modern capital city of Brazil, famed for unique architecture and city planning. After a half-day guided motorcoach tour of Brasilia we reboard our jet for the two-hour flight to Rio de Janeiro. Those participants who wish may then attend the IUPAC Macromolecular Symposium at Rio July 26-31, which will especially honor Prof. Carl S. Marvel of Illinois/Arizona. Also optional for charter flight participants will be a guided tour of Brazil from August 1-6, including Salvador de Bahia, Belo Horizonte, and Ouro Preto. The charter flight will return to Miami and New York August 6, 1974 perhaps via a stopover in Manaus, rubber center of the upper Amazon, and perhaps with a short jungle tour there.

The round-trip flight to Rio de Janeiro, the U.S. departure tax, the extra cost of the Miami and Brasilia (Manaus?) landings, the tour of Brasilia, cancellation insurance, a flight bag, reasonable baggage allowance, all meals in flight, and continuous open bar are all included for an estimated price of \$285 (about half the normal price). As always, any unexpended funds will be returned to the participants during the flight. Anyone may cancel at any time prior to flight and be reimbursed minus a nominal service charge for administrative expenses.

Any member or affiliate member of the Polymer Division plus members of their immediate families who can state that they live at the same address are eligible to participate in this Charter Flight. Members of the ACS may become full members (\$5), others may become affiliate members (\$9) by writing to Prof. James E. Mark, Chemistry Dept., University of Michigan, Ann Arbor, Michigan 48104.

To become a participant in the ACS Polymer 1974 Brazil Charter Flight, one should send names, addresses, and \$100 deposit per seat to: Dr. Henry Z. Friedlander, c/o Specialized Travel, 111 High Ridge Road, Stamford, Connecticut 06905, tel: (203)327-1781 or (212)TY3-4455. Since children occupy a full seat, they are charged full price. Checks should be made payable to ACS Polymer 1974 Brazil. Specialized Travel will assist participants in making hotel reservations, individual tours, or any other arrangements. Additional information will be forthcoming upon receipt of deposit. Remember that participants in the Charter Flight need not attend the IUPAC meeting, but one may presume some income tax advantages in doing so.

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Name (Please print or typewrite) Affiliation

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

**Return by Friday preceeding next meeting.

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