

Vol. 11, No. 8

Raleigh, N.C.

April 1981

MEETING-IN-MINIATURE

at

Duke University Durham, North Carolina

APRIL 17, 1981

PLENARY LECTURE

by

DR. R. STEVEN BERRY
University of Chicago

FROM THE ACS SAFETY COMMITTEE

The North Carolina section of the ACS announces the formation of a safety committee. One of the committee's goals will be to provide information on publication and/or knowledgeable sources on laboratory safety and chemical hazards.

Your safety questions should be brought to the attention of co-chairpersons:

Carolyn Foust at R.T.I. 541-6671 or Michael Rose at Cutter 533-5011 ext. 388.

If you share our interest in this effort, we invite you to become a member of the committee by contacting either Carolyn or Michael. Present members of the committee include Paul Greer, Henry Heck, James Bonk and Virgil Styles.

PARKING FOR THE MEETING-IN-MINIATURE

Park in any parking zone near Gross Chemical Laboratory. If ticketed, submit the ticket to the Chemistry Department office. ************

MEETING - IN - MINIATURE

at

Duke University

Durham, North Carolina

April 17, 1981



Sponsored by
The North Carolina Section

of

The American Chemical Society

PLENARY LECTURE

Room 103 Gross Chemical Laboratory

4:00 p.m.

"Finite Time Thermodynamics"

by

Dr. R. Steven Berry

University of Chicago

Presentations: 1:00 Program Enclosed

Refreshments: 2:20

& Lobby Gross Chemical Lab

3:30

Plenary Lecture: 4:00 Room 103 Gross Chemical Lab

Dinner: 6:00 A formal banquet has not

been planned. Please contact Ms. MacLeod or Dr. Gutknecht during the afternoon if you wish to accompany the speaker to

dinner.

ANALYTICAL CHEMISTRY I

C. W. Anderson, Presiding Room 110, Gross Chemical Laboratory

- 1:20 Multinuclear NMR Study of Three Aqueous Lanthanide Shift Reagents: Complexes with EDTA and Axially Symmetric Macrotyclic Polyaminopolyacetic Ligands, Charles C. Bryden, Jean F. Desreax and Charles N. Reilley, University of North Carolina-Chapel Hill.
- 1:40 PH₃ Interference on Group VIA Elements in Atomic Spectroscopy, Gary L. Long and Charles B. Boss, North Carolina State University.
- 2:00 Development of a Low Power Microwave Induced Plasma for Elemental Analysis by Atomic Emission Spectroscopy, Lawrence G. Matus and Charles B. Boss, North Carolina State University.
- 2:20 Break
- 2:30 Chemical Derivatization to Enhance ESCA Analysis of Specific Functional
 Groups on Modified Polymer Surfaces, Dennis S. Everhart and Charles N.
 Reilley, University of North Carolina-Chapel Hill.
- 2:50 A Microcomputer Compatible Mass Spectral Compression/Search Algorithm, S. J. Foulk, R. B. Lam, and T. L. Isenhour, University of North Carolina-Chapel Bill.
- 3:10 Microcomputer Based Binary-Coded Search Systems for Infrared, Carbon-13
 NMR, and Mass Spectral Data, *Alan P. Uthman, *Jerry P. Koontz, *Judy
 Hinderliter-Smith, *W. Stephen Woodward, *Charles N. Reilley, *University
 of North Carolina-Chapel Hill, *Burroughs Wellcome Company
- 4:00 Plenary Lecture

ANALYTICAL CHEMISTRY II

W. L. Switzer, Presiding Room 111, Gross Chemical Laboratory

- 1:20 Evaluation of the Area Overlap Method for Determining Adequate Chromatographic Resolution, Joseph E. Knoll and M. Rodney Midgett, U.S. Environmental Protection Agency.
- 1:40 Ion Exchange Properties of Crown Ether-Phosphotungstate Precipitates, K. K. Luk and L. H. Bowen, North Carolina State University.
- 2:00 Development of a Method for Sampling and Analysis of Metal Fumes, W. F. Gutknecht, M. B. Ranade, P. M. Grohse, and A. S. Damle, Research Triangle Institute.
- 2:20 Break

- 2:30 Ion Exchange Determination of Natural Water Organic Metal Complexing Capacities, A. Gaskill, Jr. and P. M. Grohse, Research Triangle Institute.
- 2:50 Evaluation of HPLC and IC Methods for Measurements of Organic Acids in FCD Wastes, A. Gaskill, Jr., C. M. Sparacion, E. D. Estes, A. R. Turner, J. D. Albert, S. E. Frazier and C. A. Homzak, Research Triangle Institute.
- 3:10 Surface Characterization of Pt Electrodes Using UPD of H and Cu, <u>Carey L</u>. Scortichini and Charles N. Reilley, University of North Carolina-Chapel Hill.
- 4:00 Plenary Lecture

ENVIRONMENTAL CHEMISTRY

R. K. M. Jayanty Room 103, Gross Chemical Laboratory

- 1:00 Analysis of Pesticide Reference Standards, Herman A. Krebs, U.S. Environmental Protection Agency.
- 1:20 Exposure Assessment Using Direct and Indirect Chemical Methods An Overview, D. W. Bristol, D. E. Bradway, H. L. Crist, T. R. Edgerton and K. E. MacLeod, U.S. Environmental Protection Agency.
- 1:40 Indirect Chemical Methods for Exposure Assessment, T. R. Edgerton, W. Scott, D. W. Bristol and R. E. Linden, U.S. Environmental Protection Agency and North Carolina State University.
- 2:00 Contamination Introduced During Sampling of Blood for Residue Analysis: I. Organophosphorus Compounds, <u>Diane E. Bradway</u>, <u>Douglas W. Bristol and William McDonnell</u>, U.S. Environmental Protection Agency.
- 2:20 Break
- 2:30 Contamination Introduced During Sampling of Blood for Residue Analysis: II. Organochlorine Compounds, H. L. Crist, D. W. Bristol and W. F. McDonnell, U.S. Environmental Protection Agency.
- 2:50 Development of Soil as a Quality Assurance Standard Reference Material and the Comparison of Two Soil Extraction Methods, E. J. Kantor and R. R. Watts, U.S. Environmental Protection Agency.
- 3:10 Simultaneous Determination of n-Hexane, 2-Butanone and their Metabolites in Rats by GC/MS, <u>Earl L. White</u> and James S. Bus, Chemical Institute of Toxicology.
- 3:30 Measurement of Nitric Acid and Nitrates in the Atmosphere, Robert W. Shaw, U.S. Environmental Protection Agency.
- 4:00 Plenary Lecture

GENERAL/INORGANIC/BIOCHEMISTRY

W. F. Gutknecht, Presiding Room 104, Gross Chemical Laboratory

- 1:00 Chemists to Name Buildings After: Venable, Dabney, Withers and the North Carolina Agriculture Experiment Station, Maurice M. Bursey, University of North Carolina-Chapel Hill.
- 1:20 NMR Studies of Possible Interactions of Trialkyl Tin Compounds with Biological Materials, Ronald E. Block, Nancy K. Wilson, and John T. Wilson, U.S. Environmental Protection Agency.
- 1:40 Monitoring Disorders of the Transplanted Kidney by Measuring Beta-2 Microglobulin and Other Macromolecules, D. T. Forman and S. L. Forman, North Carolina Memorial Hospital.
- 2:00 Intramolecular Electron Transfer in Organic Molecules, K. A. Goldsby and T. J. Meyer, University of North Carolina-Chapel Hill.
- 2:20 Break
- 2:30 Exchange Equilibria Studies of Crown Ether Complexed Ion Pairs in Chloroform Using Circular Dichroism, David H. Metcalf, Richard A. Palmer and Robert G. Ghirardelli, Duke University.
- 2:50 The Reaction of Boron Trifluoride with Carbon Monoxide, Geoffrey A. Blake, William L. Luken and Richard L. Wells, Duke University.
- 3:10 Thin Film Electrochemistry of Ruthenium (II) Metallopolymers, Jeffrey M. Calvert and Thomas J. Meyer, University of North Carolina-Chapel Hill.
- 3:30 The Influence of Ligand Electronic Effects on the Aquation Rates of Monohydroxamatoiron (III) Complexes, K. Poth Brink and A. L. Crumbliss, Duke University.
- 4:00 Plenary Lecture

POSTER SESSION

Lobby, Gross Chemical Laboratory

Rate Limiting Proline Isomerization in the Protein Folding of Carbonic Anhydrase, Rita A. Sheffey and Robert W. Henkens.

ESR Study of δ -CH Alkoxyl-Proton Couplings in α -Alkoxycarbonyl Radicals, Kerry K. Karukstis and Peter Smith.

ORGANIC CHEMISTRY

P. W. Jeffs, Presiding Room 105, Gross Chemical Laboratory

- 1:00 Asymmetric Synthesis of Highly Enantiomerically Pure Ethylmethyl-n-Propylcarbinol, Joseph E. Lynch and Ernest L. Eliel, University of North Carolina-Chapel Hill.
- 1:20 Neighboring Group Participation Involving Four-Membered Sulfur-Containing Rings, David E. Knox and Ernest L. Eliel, University of North Carolina-Chapel Hill.
- 1:40 Does Neighboring Group Participation Occur Through Four-Membered Oxygen-Containing Rings?, Leigh E. Clawson and Ernest L. Eliel, University of North Carolina-Chapel Hill.
- 2:00 Generation and Dipolar Addition Reactions of 2,3-Dimethyl-4-phenyloxazolium 5-Oxide, Lorraine T. Scott and John A. Hyers, North Carolina Central University.
- 2:20 Break
- 2:30 A New Synthesis of 1-Azaadamantane Derivatives, George H. Wahl, Jr. and Susan E. Zemyan, North Carolina State University.
- 2:50 Synthesis and Properties of Bicyclic Diaziridine Compounds, Robert A. Izydore and Robert Cummings, North Carolina Central University.
- 3:10 A New Class of Crown Ether Complexes Reaction of Crown Ethers with Heteropolyanions, C. A. Sporik, M. L. Miles, K. K. Luk and L. H. Bowen, North Carolina State University.
- 4:00 Plenary Lecture

PHYSICAL CHEMISTRY

W. L. Luken, Presiding Room 107, Gross Chemical Laboratory

- 1:40 Virtual Orbitals for Configuration Interaction Calculations, Barbara A.B. Seiders and William L. Luken, Duke University.
- 2:00 New Techniques for Calculating Localized Orbitals, <u>Joseph M. Leonard</u> and William L. Lukes, Duke University.
- 2:20 Break
- 2:30 Why Does the R Ton Exist?, Steve Jack, Erskine College.
- 2:50 Spin Exchange and the Triplet Exciton ESR Am = 2 Transition, D. B. Chesnut and M. A. Brown, Duke University.
- 3:10 Electron Correlation and the Chemical Bond, David N. Beratan and William L. Lukea, Duke University.
- 4:00 Plenary Lecture

- Apr 8 Dr. LOUIS S. HARRIS, Virginia Commonwealth Paiversity, "The Search for a Non-addicting Analgesic," 13th Annual Walter H. Hartung Memorial Lecture, 7:30 pm, Room 111, Beard Hall, UNC-CH.
 - 12 Dr. PAUL von RAGUE SCHLEYER, Universität Erlangen-Nürnberg, "Structural and Energetic Relationships of Lithium Reagents," 3:30 pm, Room 103 Gross Chemical Laboratory, Duke.
 - Dr. GABRIEL SAUCY, Hoffmann-LaRoche, Inc., "Synthetic Approaches to d-α-Tocopherol (Vitamin E)", 3:30 pm, Room 103 Gross Chemical Lab, Duke.
 - Dr. PAUL von RAGUE SCHLEYER, Universität Erlangen-Nürnberg, "How to Violate All Conventional Structures of Carbon Compounds," 11 am, Room 321 Dabney Hall, NCSU.
 - Dr. R. STEPHEN BERRY, University of Chicago, "Finite-Time Thermodynamics," Plenary Lecture, ACS Meeting-in-Miniature, Room 103 Gross Chemical Laboratory, Duke.
 - 23 Dr. JOANNE M. RAVEL, University of Texas at Austin, "Imitation of Protein Biosynthesis in Eukaryotes," 11:00 am, 308 Venable Hall, UNC-CH.
 - Dr. PAUL J. KROPP, University of North Carolina-Chapel Hill, "Photo-chemistry of Alkyl Halides: A Convenient and Powerful Method for Generation of Carbocations," 3:30 pm, Room 103 Gross Chemical Lab, Duke.
 - 27 Dr. NED ARNETT, Duke University, "Solvation Energies: The Missing Link in Organic Chemistry," 3:30 pm, Room 124 Dabney Hall, NCSU.
- May 14 Dr. ALEXANDER I. POPOV, Michigan State University, Title to be announced, 3:30 pm, Room 103 Gross Chemical Laboratory, Duke.

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