## Rocky Mountain Conference on Magnetic Resonance

Volume 33 33rd Rocky Mountain Conference on Applied Spectroscopy

Article 1

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## 33rd Rocky Mountain Conference on Applied Spectroscopy

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### 33rd Rocky Mountain Conference on Applied Spectroscopy

#### Abstract

Program and registration information for the 33rd annual meeting of the Rocky Mountain Conference on Applied Spectroscopy, sponsored by the Rocky Mountain Section of the Society for Applied Spectroscopy. Held in Denver, Colorado, July 28 - August 1, 1991.

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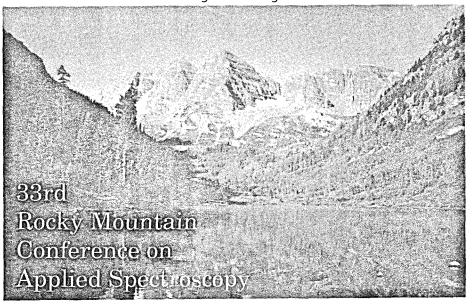


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et al.: 33rd RMCAS Program and Registration Information



# PROGRAM AND REGISTRATION INFORMATION

JULY 28 - AUGUST 1, 1991

RADISSON HOTEL DENVER 1550 COURT PLACE DENVER, COLORADO

SPONSORED BY

ROCKY MOUNTAIN SECTION SOCIETY FOR APPLIED SPECTROSCOPY

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#### SYMPOSIA SCHEDULE (Page Number in Program)

Monday Tuesday Wednes. Thur.
July 29 July 30 July 31 Aug. 1

|  | am | pm | am | pm | am | pm | am |
|--|----|----|----|----|----|----|----|
| Atomic Spectroscopy                        |    |    | 18 | 18 |    |    |    |
| Electrochemistry                           | 19 | 20 | 21 |    |    |    |    |
| Environmental Chemistry                    |    |    | 21 | 22 | 23 |    |    |
| EPR Symposium                              | 24 | 24 | 25 | 25 | 28 | 29 | 32 |
| FTIR/NEAR-IR                               | 32 |    |    |    |    |    |    |
| Gas, Ion & Supercritical<br>Chromatography | 33 |    |    |    |    |    |    |
| Luminescence                               |    |    | 34 | 34 |    |    |    |
| Mass Spectrometry                          | 35 | 35 |    |    |    |    |    |
| NMR  | 36 | 36 | 37 | 38 | 38 | 38 | 39 |
| Quality Assurance                          |    | 40 |    |    | 41 | 42 |    |
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#### CONFERENCE LOCATION

Technical sessions and the exhibition for the 33rd Rocky Mountain Conference on Analytical Chemistry will be held in the Radisson Hotel Denver, 1550 Court Place, Denver, Colorado.

#### REGISTRATION

Admission to all technical sessions and the exhibition is by the name badge for the 33rd Rocky Mountain Conference. Preregistration, using the form in the center of this booklet, is encouraged. The deadline for the receipt of the preregistration form and full remittance of conference fees is July 20, 1991. Conference fees are payable by check (denominated in \$US, only) made payable to the Rocky Mountain Conference.

#### Registration Fees - 1991

|                                    | Preregistrat | ion On Site    |
|------------------------------------|--------------|----------------|
|                                    | (received by | July 21, 1991) |
| Registration                       | \$60.00      | \$80.00        |
| Registration (one specified day)   | 35.00        | 45.00          |
| Student Registration               |              | 15.00          |
| Additional Vendor registration     |              | 45.00          |
| Unemployed or retired registration | on           | 15.00          |
| Exhibition only (non-vendor)       |              | 10.00          |

#### Refunds

Requests for refunds of conference fees must be received by July 20, 1991.

#### <u>Times</u>

On-site registration for the 33rd Rocky Mountain Conference will be held in the Convention Lobby of the Radisson Hotel Denver during these times:

| Sunday, July 28    | 5:00 p.m9:00 p.m.  |
|--------------------|--------------------|
| Monday, July 29    | 7:30 a.m3:30 p.m.  |
| Tuesday, July 30   | 7:30 a.m3:30 p.m.  |
| Wednesday, July 31 | 7:30 a.m3:30 p.m.  |
| Thursday, August 1 | 8:00 a.m10:00 a.m. |

#### EXHIBITION

The Rocky Mountain Conference exhibition provides an opportunity to see and discuss the latest in analytical instrumentation, supplies, and services. Other activities in the exhibition hall include coffee breaks, mixers and poster sessions.

#### Hours

| Sunday, July 28    | Mixer     | 7:00 p.m9:00 p.m. |
|--------------------|-----------|-------------------|
| Monday, July 29    | Exhibits  | 9:30 a.m5:00 p.m. |
| Monday, July 29    | Posters   | 2:00 p.m4:00 p.m. |
| Monday, July 29    | Reception | 5:00 p.m7:30 p.m. |
| Tuesday, July 30   | Exhibits  | 9:30 a.m5:00 p.m. |
| Wednesday, July 31 | Exhibits  | 9:30 a.m5:00 p.m. |

Posters will be set up in the exhibition area Monday morning through Wednesday afternoon.

For space or information about the exhibition, contact:

Jim Parker R-38 Manville Technical Center 10100 West Ute Avenue Littleton, Colorado 80127 TEL (303) 978-5481 FAX (303) 978-5094

The following have reserved space as of April 17, 1991:

Allen Scientific Glass Blowers Analytical Science, Inc. Bruker Instruments Cenref Laboratories COSA INSTRUMENT CORP. Finnigan MAT General Air Service & Supply Huffman Laboratories Laboratory MicroSystems Medical Advances, Inc. Oxford Instruments N. America PUREGAS - General Cable Company Resonance Research Tekmar Company Thermo Jarrell Ash Waters Division of Millipore Western Analytical Instrumentation

Analytical Development Corp. Applied Technical Products CEM Corporation Chemagnetics Doty Scientific FISONS/ARL GMW Associates JEOL U.S.A., Inc. LECO Corporation Micro-Now Instrument, Co. Perkin Elmer Questron Corporation SiWest Company Telecation Associates Varian Instrument Group Wilmad Glass Company

Time and space are also available for exhibitors interested in sponsoring short workshops. Please contact Glenda Brown for more information.

#### Social Program

#### Registration Night Mixer

A cash bar will be open in the conference registration area of the Radisson Hotel Denver on Sunday evening, July 28, from 7:00 to 9:00 p.m. Plan to meet other conference attendees and beat the Monday rush to pick-up your conference badge and abstract book.

#### Conference Mixer

On Monday afternoon, July 29, immediately after the conference, please join us for a cocktail and hors d'oeuvre mixer at the Radisson Hotel in the Exhibit area.

#### Conference Banquet

The conference banquet will be on Tuesday, July 30, at 7:00-10:00 p.m. in the Majestic Ballroom of the Radisson. Tickets are \$28 each. There will be a cash bar in the Majestic Lounge at 6:00 p.m.

Our banquet speaker this year is Dr. John Firor, a distinguished scientist and one of the founders of the National Center for Atmospheric Research. Dr. Firor is physicist by training and has held faculty positions at a number of universities. He is a trustee of the World Resources Institute, the Environmental Defense Fund, NASA Space and Terrestrial Applications Board, and CU's Natural Resources Law Center.

Dr. Firor is pioneer in the area of global warming and the greenhouse effect. In his presentation, he will help us sort out the facts, speculation, misconceptions, politics and science of global climatology, one of the most significant environmental matters facing our planet.

#### TOUR

On Wednesday, July 31, there will be a guided tour (approximately 30 minutes) of the operating brewery at the Wynkoop Restaurant located in historic downtown Denver, followed by dinner at the Wynkoop. The tour if free, but there is an additional charge for beer and food consumed. Space is limited, so please make your reservations early, before June 15. Contact Bob Conway, P.O. Box 6167, Denver, CO 80206. Phone: (303) 624-4174, FAX (303) 624-3384.

#### TRAVEL

#### Special Rocky Mountain Conference Fares on Continental Airlines

Continental Airlines has joined with the Rocky Mountain Conference to offer special airfares that are not available to the general public when you attend the conference and travel between July 23, 1991 and August 8, 1991. inclusive.

- A) Continental Airlines will offer a variety of discount fares, call for availability. To obtain these special fares follow these easy steps:
- Phone Continental at 800-468-7022. Call weekdays 6:00 a.m. to 12:00 midnight, CST, and Saturdays from 8:00 a.m. to 4:00 p.m., CST.
- The identification number assigned to the Rocky Mountain Conference is EZ7P50.
- 3. Continental specialists will provide information and make reservations for all flights and fares, including the special conference fare. The special Rocky Mountain Conference fare is available on Continental flights within the United States (in Canada, ask for the special meeting fare).

Whichever means of ticketing you choose, the special conference fare can only be obtained when the reservation is initiated by phone through the special Continental 800 number listed above.

Seats are limited, so call early for best availability. Fares are guaranteed at time of ticket purchase. Tickets must be requested two weeks in advance of desired travel. Tickets may not be sold or bartered.

#### HOUSING

#### Hotel Accommodations

Hotel rooms at the Radisson Hotel Denver, 1550 Court Pl., Denver, CO 80202, (303) 893-3333, are available at the guaranteed conference rate of \$80 per night (single), \$90 per night (double), plus applicable tax. Suites available upon request at the conference discount. The reservation form in the center of the booklet must be returned directly to the hotel.

Additional hotels, within easy walking distance or a short ride on a 16th Street Mall shuttle bus (free), are listed below. Locations are given on the map inside the back cover. For rates and reservations, contact the hotel directly.

The Brown Palace Hotel, 321 17th St., Denver, CO 80202, (303) 297-3111 or 800-321-2599 (800-228-2917 in Colorado).

Comfort Inn, 401 17th St., Denver, CO 80202. (303) 296-0400, 800-631-2090 (Colo), 800-237-7431 (outside Colo).

Executive Tower Inn, 1405 Curtis St., Denver, CO 80202, (303) 571-0300 or 800-525-6651.

Hyatt Hotel, 1750 Welton St., Denver, CO 80202, (303) 295-1200 or 800-527-4727.

Hotel Denver-Downtown, 1450 Glenarm Pl., Denver, CO 80202, (303) 573-1450 or 800-423-2201 (Colo), 800-423-5128 (outside Colo)..

Marriott City Center, 1701 California St., Denver, CO 80202, (303) 297-1300 or 800-228-9290.

Warwick, 1776 Grant St., Denver, CO 80203, (303) 861-2000 or 800-525-2888.

Low cost student housing is also available at local universities. Commute time to the conference site ranges from 20 to 45 minutes via regional bus transportation. For rates and reservation information, contact Joe Broadus at (303) 236-5345.

#### ADDITIONAL ACTIVITIES

#### Visitor Information

Denver and the surrounding area boast a large number of activities that are enjoyable for both young and old. For additional information contact the Denver Metro Convention and Visitors Bureau, 225 W. Colfax Ave., Denver, CO 80202, (303) 892-1112. For information about statewide attractions contact the Colorado Tourism Board, 1625 Broadway, Suite 1700, Denver, CO 80202, (303) 592-5510.

#### Employment Clearing House

The employment committee of the Colorado Section of the American Chemical Society will sponsor an employment clearing house. Resumes will be accepted prior to, and during the meeting, for review by prospective employers. Facilities will be available for on-site interviews by employers. Employers and job-seekers interested in early registration should contact one of the employment committee members listed below by July 15, 1991.

Douglas B. Manigold, Chairman U.S. Geological Survey 5293 Ward Road Arvada, CO 80002 (303) 236-5345 FAX (303) 467-9598

Helen Brandenburg U.S. Geological Survey 5293 Ward Road Arvada, CO 80002 (303) 236-5345 FAX (303) 467-9598 Sonia Atwood Marathon Oil Company P.O. Box 269 Littleton, CO 80160 (303) 794-2601 FAX (303) 794-1720

Ronald G. Thompson Marathon Oil Company P.O. Box 269 Littleton, CO 80160 (303) 794-2601 ext. 708 FAX (303) 794-1720

Interested employers and job seekers can receive additional information on available jobs and on the employment booth activities by calling the ACS Employment committee Hotline number which is (303) 933-4375.

#### Message Center

Incoming telephone messages for conferees will be posted at the message center in the registration area. The telephone is (303) 893-3333, ext. 337. Ask for the Rocky Mountain Conference message center. This service will be available from 8:00 a.m. to 3:30 p.m. Monday-Wednesday and from 8:00 a.m. to 10:00 a.m. Thursday.

#### Restaurant Service

The Communications Department of the Denver Metro Convention and Visitors Bureau will provide a FREE restaurant service designed to let out-of-town delegates know about Denver's world class dining opportunities, from casual to elegant. The Dining Desk will have a header that reads "Free Restaurant Reservations", and will also have an experienced reservation person, a phone and a cart featuring poster-size menus that delegates can browse through. This service has been in operation for five years and has been extremely successful in providing delegates with convenient, courteous, and efficient service.

# SHORT COURSES (Sponsored by the Colorado Section of the ACS)

The Education Committee of the Colorado Section of the ACS is offering short courses in conjunction with the 33rd Rocky Mountain Conference as described below. Registration forms are included following this page. The Radisson Hotel Denver has agreed to provide lodging for short course participants at the special conference rate. Please mention the 33rd Rocky Mountain Conference when making reservations. All courses will be taught at the University of Colorado at Denver, in downtown Denver. Tuition will be refunded if course registration is cancelled before July 15, 1991.

#### QUALITY ASSURANCE PRACTICES FOR THE ENVIRONMENTAL LABORATORY

Steve Callio

2 days: August 1-2, 1991

Tuition: member \$350; non-member \$400

#### AIR POLLUTION CHEMISTRY

Dr. Donald H. Stedman

2 days: August 1-2, 1991

Tuition: member \$350; non-member \$400

# BASIC FRINCIPLES OF MASS SPECTROMETRY AND INTERPRETATION OF ORGANIC MASS SPECTRA

OR

Dr. J.A. Zirrolli

3 days: July 31, August 1-2, 1991 Tuition: member \$400; non-member \$450

Registration deadline for all courses is July 15, 1991. For more information contact:

Dr. Joesph A. Zirrolli National Jewish Center Dept. of Pediatrics, K923 1400 Jackson Street Denver, CO 80206 TEL 303-398-1136 FAX 303-398-1694 Marilyn Johnsen University of Denver Dept. of Chemistry Denver, CO 80208 TEL 303-871-2580 FAX 303-871-2587

# SHORT COURSE REGISTRATION Courses Sponsored by Colorado Section American Chemical Society at the 33rd Rocky Mountain Conference Denver, Colorado

Member Non-Member (ACS, SAS, RMCDG) Quality Assurance Practices for the Environmental Laboratory **□\$350 □\$400** August 1-2, 1991 Air Pollution Chemistry **□\$350** August 1-2, 1991 **□\$400** Basic Principles of Mass Spectrometry and Interpretation of Organic Mass Spectra **□\$400** D\$450 July 31, August 1-2, 1991 Organization: Address: City, State, Zip: \_\_\_\_\_FAX:\_\_\_\_\_ Refund Policy: Full refunds will be made if requests are received on or before July 15, 1991. Make checks payable to "Colorado Section ACS" and send payment with this form to:

> Dr. Joseph A. Zirrolli Dept. of Pediatrics K923 National Jewish Center 1400 Jackson Street Denver, CO 80206

Phone: (303) 398-1136 FAX: (303) 398-1694

#### SHORT COURSES

(Sponsored by the Colorado Section of the ACS)

#### QUALITY ASSURANCE PRACTICES FOR

THE ENVIRONMENTAL LABORATORY

Instructor: Steve Callio

August 1-2, 1991

Tuition: \$350 member; \$400 non-member

This two day short course is designed for laboratory analysts who require an introduction to quality assurance practices used in environmental measurements. The course starts with a discussion of basic statistical concepts required in QA, i.e., detection limits, confidence limits, determination of standard deviations; then the principles of quality assurance are explained and discussed in depth. These range from the preparation of duplicate and spiked samples, use of internal standards and standard reference materials, and instrument calibration to the role of the QA manager, training requirements and record documentation. Examples of the application of these procedures to actual environmental analyses; BOD, solids analyses, colorimetric procedures (nitrate, phosphate), ICP of metals, GC analyses; residual chlorine and fluoride determinations are then discussed.

In addition to laboratory analysts, engineers and project officers who use laboratory-generated data in their programs and require a better understanding of how the data are obtained, will benefit from this course.

Faculty: Steve Callio, B.S., M.S., has more than 15 years of experience in Environmental Analytical Chemistry. He has worked with government and private testing laboratories and in the Laboratory Quality Assurance field. He has presented papers to EPA's Contract Laboratory Program, the Symposium on Solid Waste Testing and published with ASTM and Atomic Spectroscopy. This course was well received when it was presented for the first time last year.

For Short Course Registration by July 15, 1991 use the form preceding course descriptions. For more information contact:

OR

Dr. Joseph A. Zirrolli National Jewish Center Dept. of Pediatrics K923 1400 Jackson Street Denver, CO 80206 TEL 303-398-1136 FAX 303-398-1694 Marilyn Johnsen University of Denver Dept. of Chemistry Denver, CO 80208 TEL 303-871-2580 FAX 303-871-2587

# SHORT COURSES (Sponsored by the Colorado Section of the ACS)

AIR POLLUTION CHEMISTRY

Instructor: Dr. D.H. Stedman

August 1-2, 1991

Tuition: \$350 member: \$400 non-member

This course uses the concepts of Chemical Thermodynamics, Chemical Kinetics, and Photochemistry to understand the processes which give rise to polluted air. The course begins with an analysis of combustion systems and other pollution sources. The analysis continues by describing the chemical reactions which occur in air near to the source, in the air in the region of the source and in the air a long way downwind from the source. Problems to be worked by the students and an overnight homework experiment which can be performed in a hotel room are included. Depending on student interest a section of air pollution measurement techniques may be substituted for the section on stratospheric pollution and the ozone hole.

Faculty: Dr. Donald H. Stedman is the Brainerd F. Phillipson Professor of Chemistry at the University of Denver. He is a noted expert in air pollution chemistry with over 20 years experience and over 150 publications in Atmospheric Chemistry, Chemical Kinetics, Trace Analysis and Chemiluminescence. He is a member of the American Chemistry, the Air Pollution Control Association, and the American Association for the Advancement of Science.

For Short Course Registration by July 15, 1991 use the form preceding course descriptions. For more information contact:

OR

Dr. Joseph A. Zirrolli National Jewish Center Dept. of Pediatrics K923 1400 Jackson Street Denver, CO 80206 TEL 303-398-1136 FAX 303-398-1694 Marilyn Johnsen University of Denver Dept. of Chemistry Denver, CO 80208 TEL 303-871-2580 FAX 303-871-2587

# SHORT COURSES (Sponsored by the Colorado Section of the ACS)

#### BASIC PRINCIPLES OF MASS SPECTROMETRY AND INTERPRETATION

OF ORGANIC MASS SPECTRA

Instructor: J.A. Zirrolli, Ph.D.

July 31, August 1,2, 1991

Tuition: \$400 member: \$450 non-member

This three day course will describe the principles of modern mass spectrometry and apply them to the identification of organic compounds. Sample introduction methods (GC, LC, vapor, direct probe), ionization processes (positive, negative, FAB, chemical, electronic), mass analysis and detection will be discussed with emphasis on molecular ion analysis and simple fragmentation processes. The course will develop an approach to the determination of elemental composition and diagnostic fragmentation patterns, and the student will become familiar with the mass spectra characteristic of common organic compound classes, drugs, pesticides and pollutants. The course is based upon and uses as a reference the text, Interpretation of Organic Mass Spectra, Third Edition by F.W. McLafferty, University Science Books, 1980, which will be provided.

<u>Faculty</u>: Dr. Joseph A. Zirrolli is a Research Associate in the Department of Pediatrics and Research Director of the Mass Spectrometry Center at the National Jewish Center for Immunology and Respiratory Medicine at Denver. He is a member of the American Chemical Society and the American Society of Mass Spectrometry.

For Short Course Registration by July 15, 1991 use the form preceding course descriptions. For more information contact:

Dr. Joseph A. Zirrolli National Jewish Center Dept. of Pediatrics K923 1400 Jackson Street Denver, CO 80206 TEL 303-398-1136 FAX 303-398-1694

Marilyn Johnsen
University of Denver
Dept. of Chemistry
OR Denver, CO 80208
TEL 303-871-2580
FAX 303-871-2587

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#### Environmental Seminar

9:00 a.m. to 12:00 p.m., Thursday, August 1, 1991

Waters Chromatograph Division is offering a half-day seminar covering areas of interest to environmental chemists. The day will focus on understanding the various methodologies and the results one can expect from "real world" samples. The seminar will cover:

Method set-up and instrumentation requirements. Chromatographic separations with standard and samples shown on data stations.

Expectations for Minimum Detectable Level and Reproducibility.

The following special interest areas will be reviewed:

GPC Sample Clean-up
Carbamate and Glyphosate Residues
Polyaromatic Hydrocarbons
Anions
Solid Phase Extraction
Analytical Laboratory Information Management
Millipore Analytical Products
Capillary Electrophoresis

The seminar is free, however registration is recommended. If additional information is required please contact Duane Mauzey at 1-800-632-2708, Ext. 152, or your local Waters Technical Representative. A confirmation letter will be sent when registration is received or simply by calling 1-800-632-2708, Ext. 162 for location/registration information.

| Name:  |         |     |                |                 |    |
|--|---------|-----|----------------|-----------------|----|
| Position:  |         |     |                |                 |    |
| Organization:  |         |     |                |                 | _  |
| Mailing Address:                                       |         |     |                |                 |    |
| City:  | _State: | ;   | Zip:           |                 |    |
| Telephone:   |         |     |                |                 | _  |
| I am currently using HPLC, my environmental laboratory | •       | ion | chromatography | instrumentation | in |
| Yes  | _       |     | _No            |                 |    |

To register, complete form and return to: Waters/Millipore Regional Office, 448 Grandview Drive, South San Francisco, CA 94080, Attn: Environmental Seminar

#### et al.: 33rd RMCAS Program and Registration Information

Everything You Always Wanted to Know About LIMS But Were Afraid To Ask

9:00 a.m. to 12:00 p.m., Thursday, August 1, 1991

Presented by: Laboratory MicroSystems, Inc.

This seminar will be of interest to those looking to implement a new LIMS, replace an existing LIMS, or who would like to find out more about LIMS in general.

Who should attend:

Lab personnel-directors, managers, technicians, etc.

Quality control personnel-supervisors, engineers, etc.

Computer information management personnel.

Anyone planning on implementing a LIMS.

Topics to be covered:

What is LIMS?

How can a LIMS benefit me?

What computers can I use for LIMS?

How does a LIMS get implemented?

There is no additional charge for this seminar, but registration is limited. For registration information, contact Dori Vallone at (518) 274-1990, or send inquiries to her at:

Laboratory MicroSystems, Inc. Hendrick Hudson Building 200 Broadway Troy, NY 12180

#### ThermoSPECTM Software Seminar

8:30 a.m. to 5:00 p.m., Thursday, August 1, 1991

A workshop for experienced users of ThermoSPECTM software for Thermo Jarrel Ash AAS and ICPES systems will be offered to Rocky Mountain Conference attendees. There is an additional \$20 charge for this workshop which will include lunch. A structured learning session, led by Ron Manabe, will be held in the morning with open discussions following the lunch break. Space will be limited for this workshop and preregistration is recommended. The deadline for onsite registration is noon on Monday, July 29, 1991. Call (415) 327-5605 if additional information is needed.

#### Seminar Topics:

- \* Version-to-version updates
- \* Use of command language
- \* Ancillary integrated software (including Enable and SPC)
- \* Turbo-ThermSPECTM
- \* Latest in preintroduction systems (chelation chemistry, ultrasonic)
- \* User open forum
- \* Group discussions
- \* Formation of User Groups

Formal presentations will begin promptly at 9:00 a.m. on Thursday, August 1, 1991.

|  | <del></del>  |
|--|--|
| ThermoSPECTM Seminar Registration Form   |  |
| Name   | Make checks payable to                                   |
| Company  | Rocky Mountain Conference                                |
| Address  |  |
|  |  |
| Phone  | This seminar is available only                           |
| to RMC attendees. The \$20 seminar fee may   | be added to your RMC                                     |
| preregistration payment.   |  |
| Please provide the following information ThermoSPEC $^{\text{TM}}$ software so we may tailor the | concerning your current use of e course to participants. |
| ThermoSPEC $^{TM}$ used on the following instru  | ments:   |
| Data manipulation and reporting packages   | used:  |
| Data are exported to the following LIMS:   |  |

#### MODERN NEAR-IR ANALYSIS

Instructor: Donald A. Burns July 27-28, 1991 Tuition: \$500

This course is intended for those with little or no previous experience with Near-IR, analytical chemists and managers who are considering entering the field, and those who are responsible for routine analyses or development of methods where speed, cost, and simplicity are important. The first day of the course will cover history, principles, theory: optics/instrumentation: data collection and manipulation (teaching and reference sets) and statistics/chemometrics. The second day of the course will cover sample selection/handling; discriminant analysis; indicator variables; online analysis; fiber optics; method development and industrial applications. The student will learn principles and instrumentation; quantitative and qualitative analysis; chemometric/multivariate techniques; solving problems in your field; and who makes what instruments. The student will also learn the benefits of fast analyses (30 seconds); little/no sample preparation; NIR: versatile (sees -CH, -OH, -C=O groups); handles liquids and solids and usable with fiber optics (remote sensing).

Faculty: Dr. Donald A. Burns is a staff scientist at Los Alamos National Laboratory. He has been involved with NIR for about ten years. He received the 1990 Eastern Analytical Symposium award for achievements in NIR, and has taught an ACS-sponsored short course in this field since 1984.

For course information . For more information contact:

Dr. Donald A. Burns
2 La Flora Court
Los Alamos National Laboratory
Los Alamos, NM 87544
TEL (505) 665-4186
FAX (505) 665-4737

#### Organizers of the 33rd Rocky Mountain Conference

- Conference Chairwoman Pat Sulik, Rocky Mountain Instrumental Labs., 456 S. Link Lane, Fort Collins, CO 80524, (303) 530-1169.
- Conference Program Chairman Steve Callio, U.S. EPA Region VIII, (303) 294-7509.
- Exhibits Jim Parker, Manville Tech Center, Mail Stop R-38, PO Box 5108, Denver, CO 80217, (303) 978-5481.
- Registration Barbara Macklin, USGS, Mail Stop 408, 5293 Ward Road, Arvada, CO 80002, (303) 236-3600. Joe Broadus, USGS, NWQL, 5293 Ward Road, Arvada, CO 80002, (303) 236-5345.
- Treasurer Glenda Brown, USGS, Mail Stop 407, 5293 Ward Road, Arvada, CO 80002, (303) 236-5345.
- Social Events Bob Conway, PO Box 6167, Denver, CO 80206, (303) 624-4174.
- Staff Glenda Brown, USGS, Mail Stop 407, 5293 Ward Road, Arvada, CO 80002, (303) 236-5345.
- Short Courses Joe Zirrolli, Dept. of Pediatrics, K923, National Jewish Center, 1400 Jackson St., Denver, CO 80206, (303) 398-1853, FAX (303) 398-1694.
- Audio-Visual Mark Brugh, EGG Rocky Flats, P.O. Box 464, Golden, CO 80402-0464, (303) 966-5217.
- Mailing List Carol Gies, EG&G Incorporated, Rocky Flats, P.O. Box 464, Golden, CO 80402, (303) 966-7380.

  Jana Dawson, EG&G Incorporated, Rocky Flats, HSE Labs., Bldg. 123, P.O. Box 464, Golden, CO 80402
- Program Typist Debbie Litwin, USGS, MS 408, 5293 Ward Road, Arvada, CO 80002, (303) 236-3609.

#### Symposia Chairwomen and Chairmen

- Atmospheric Spectroscopy Gary Rayson, Dept. of Chemistry, New Mexico State University, Las Cruces, NM 88003, (505) 646-5839.
- Electrochemistry Charles Martin, Dept. of Chemistry, Colo. State Univ., Ft. Collins, CO 80523, (303) 491-0271.
- Electron Paramagnetic Resonance Gareth Eaton, Univ. of Denver, Denver, CO 80208-0179, (303) 871-2980.

  Sandra Eaton, Univ. of Denver, Denver, CO 80208-0179, (303) 871-3102.

- Environmental Chemistry Lynda Faires, U.S. Geological Survey, Box 25046, MS 407, Denver Federal Center, Denver, CO 80225, (303) 236-9362 or 5345.
- FTIR/NEAR IR A.R. Chughtai, Dept. of Chemistry, Mudd Bldg., Univ. of Denver, Denver, CO 80208, (303) 871-4404.

  Joseph Montalvo, USDA, ARS-SRRC, P.O. Box 19687, New Orleans, LA 70179, (504) 286-4249.
- Gas, Ion and Supercritical Fluid Chromatrography Bill Williams, Manville Tech. Center, P.O. Box 5108, Denver, CO 80217, (303) 978-5595.
- General Posters Elizabeth Sexton, Analytica Inc., 18000 W. Hwy. 72, Golden, CO 80403, (303) 420-4449.
- Luminescence Marvin Goldberg, U.S. Geological Survey, P.O. Box 25046, MS 424, Lakewood, CO 80225, (303) 236-4728.
- Mass Spectrometry Joe Zirrolli, Dept. of Pediatrics, K923, National Jewish Center, Denver, CO 80206, (303) 398-1853.
- Nuclear Magnetic Resonance Hellmut Eckert, Dept. of Chemistry, Univ. of California, Santa Barbara, CA 93106, (805) 893-8163.
- Quality Assurance Bill Shampine, USGS, MS 410, Box 25046, DFC, Denver, CO 80225, (303) 236-1940.

# SYMPOSIUM ON ATOMIC SPECTROSCOPY Organized by Gary Rayson

|             | Organized by Gary Rayson  |
|-------------|---|
| Tuesday, Ju | aly 30, 1991  |
| 8:30        | <u>KEYNOTE SPEAKER</u> , NEW PLASMA SOURCES FOR ANALYTICAL ATOMIC SPECTROSCOPY. <u>M.W. Blades</u> , University of British Columbia.  |
| 9:00        | THE DETERMINATION OF TRACE METALS IN SALINE WATER BY GFAA WITH PALLADIUM MODIFICATION. John T. Creed, Larry B. Lobring, Theodore D. Martin, and James W. O'Dell, U.S. Environmental Protection Agency.                                |
| 9:20        | THERMAL PRETREATMENT SILVER ANALYTE LOSS - IMPACT OF MAGNESIUM AND PALLADIUM MODIFIERS. <u>Gary D. Rayson</u> and Mark. R. Fresquez, New Mexico State University.   |
| 9:40        | ENHANCED ICP-MS ANALYSES WITH CHEMICAL SEPARATIONS. <u>Ellyn S. Beary</u> and Paul J. Paulsen, National Institute of Standards and Technology.  |
| 10:00       | BREAK   |
| 10:30       | OPTIMIZATION AND MICROWAVE SAMPLE PREPARATION PROCEDURES VIA FEEDBACK CONTROL OF TEMPERATURE AND PRESSURE PARAMETERS. Elaine T. Hasty, Sara F. Littau, and W.G. Englehart, CEM Corporation.   |
| 10:50       | COMPARISON OF HIGH-PRESSURE SAMPLE PREPARATION APPROACHES FOR ANALYSIS BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. Ramon M. Barnes, Chitra Amarasiriwardena, Henry Foner, and Antoaneta Krushevdka, University of Massachusetts. |
| 11:10       | FRELIMINARY REPORT ON THE MODIFIED LICHTE NEBULIZER FOR INTRODUCING SAMPLES OF VARIED MATRICES INTO AN INDUCTIVELY COUPLED PLASMA. <u>Gerhard A. Meyer</u> , Battelle, Columbus, OH.  |
| 11:30       | PRELIMINARY EVALUATION OF AN INDUCTIVELY COUPLED PLASMA TORCH FABRICATED WITH A 2.5 mL VOLUME MICROSPRAY CHAMBER. Gerhard A. Meyer, Battelle, Columbus, OH.   |
| 12:00       | LUNCH   |
| 1:30        | THE COMPLETE ICP-AES PERIODIC TABLE: WILL 196 LINES SUFFICE FOR ALL APPLICATIONS? Pascal Cassagne and Robert C. Fry, Fisons Instruments.  |
| 1:50        | A COMPLETELY MODULATED SAMPLE INTRODUCTION SYSTEM FOR ATOMIC EMISSION SPECTROMETRY. Ruth E. Wolf, Rodney K. Skogerboe, and Jeffrey J. Rosentreter, FG&G Idaho, Incorporated.  |

- 2:10 A NEW ECHELLE OPTICAL DESIGN: ELIMINATION OF FOCAL PLANE RESTRICTIONS TO CREATE A 196 CHANNEL ICP-AES SPECTROMETER.
  M.W. Routh, W. Vogel, F. Pilloud, P. Cassagne, and D.F. Sermin, Fisons Instruments, Switzerland; and G.H. Gower, and R.C. Fry, Fisons Instruments, Valencia, CA.
- 2:30 THE UTILIZATION OF AN INDUCTIVELY COUPLED ARGON PLASMA AXIAL VIEWING ABSORPTION TECHNIQUE FOR THE DETERMINATION OF RARE EARTH ELEMENTS. <u>Gary D. Rayson</u> and Daniel Y. Shen, New Mexico State University.
- 2:50 BREAK
- 3:10 DEVELOPMENT AND FUNDAMENTAL CHARACTERIZATION OF AN AXIALLY VIEWED ICP WITH ELECTRON NUMBER DENSITIES EXCEEDING  $10^{16}/\mathrm{cm}^3$ . R.L. Dahlquist, R. Eldridge, D. Tasker, B. Kenessey, and R.C. Fry, Fisons Instruments.
- 3:40 HIGH ELECTRON NUMBER DENSITY AND EXTENDED RESIDENCE TIME ELIMINATE MATRIX EFFECTS AND MOLECULAR BANDS IN AN AXIALLY VIEWED ICP. R.L. Dahlquist, R. Eldridge, D. Tasker, and R.C. Fry, Fisons Instruments.
- 4:00 A REEXAMINATION OF END-ON VIEWING OF THE PLASMA DISCHARGE IN ICP-OES. <u>D. Nygaard</u>, D. Demers, T. Alavosus, and F. Bulman, Baird Corporation.

# SYMPOSIUM ON ELECTROCHEMISTRY Organized by Charles R. Martin

Monday morning, July 29, 1991

- C.R. Martin, Presiding
- 8:30: CRYSTALLINE LANGMUIR-BLODGETT FILMS ON ELECTRODE SURFACES: CHARACTERIZATION BY ELECTROCHEMISTRY AND SCANNING TUNNELING MICROSCOPY. Reginald M. Penner, University of California at Irvine.
- 9:00: MOLECULAR PROBES FOR INVESTIGATING THE LOCAL ELECTROCHEMICAL ENVIRONMENT AND ITS INFLUENCE ON REDOX TRANSFORMATIONS IN SELF-ASSEMBLED MONOLAYERS ON GOLD ELECTRODES. Sandra M. Kimbrell, and Daniel A. Buttry, University of Wyoming.
- 9:30: IMAGING OF DEFECTS CONTAINED WITHIN N-ALKYLTHIOL MONOLAYERS
  BY COMBINATION OF UNDERPOTENTIAL DEPOSITION AND SCANNING
  TUNNELING MICROSCOPY: KINETICS OF SELF-ASSEMBLY. Richard M.
  Crooks, and Li Sun, University of New Mexico.
- 10:00: A STUDY OF ELECTRON AND SOLVENT TRANSPORT THROUGH MONOLAYERS
  OF VIOLOGENS CONTAINING FLUOROCARBON CHAINS, Shauna L.
  Hiley, and Daniel A. Buttry, University of Wyoming.

10:30: BREAK

10:45: DENSITIES, MOLAR VOLUMES AND EXPANSIVITIES IN ROOM TEMPERATURE CHLOROALUMINATE MOLTEN SALTS. Anselmo M. Elias

and John S. Wilkes, U.S. Air Force Academy.

11:15: ELECTROCHEMICAL CHARACTERIZATION OF A SERIES OF TRIPLY BRIDGED DINUCLEAR TRIS(BIPYRIDINE) IRON COMPLEXES. C.

Michael Elliott, Sue Ferrere, Barbara R. Serr, and Kevin

Andersen, Colorado State University.

11:45: LUNCH

R.M. Crooks, Presiding

1:30: CONDUCTING POLYMER ULTRATHIN FILM COMPOSITE MEMBRANES BY INTERFACIAL DEPOSITION AND A NEW APPROACH FOR GAS

SEPARATION. Wenbin Liang, and Charles R. Martin, Colorado

State University.

2:00: THE USE OF ELECTROPOLYMERIZED METALLOPORPHYRIN FILMS FOR THE

SEPARATION OF NITROGEN HETEROCYCLES FROM HYDROCARBON PHASES VIA ELECTROCHEMICALLY MODULATED COMPLEXATION. Douglas E.

Wedman and Carl A. Koval, University of Colorado.

2:30: A STUDY OF THE CHARGE TRANSFER MECHANISM IN ELECTRONICALLY

CONDUCTING POLYMER COMPOSITE SEPARATOR MEMBRANES. <u>Del R.</u> <u>Lawson</u>, Wenbin Liang, Edward Z. Cai, and Charles R. Martin,

Colorado State University.

3:00: BREAK

3:15: THE PHOTODEPOSITION OF METALS AT SINGLE CRYSTAL AND

PARTICULATE TITANIUM DIOXIDE SEMICONDUCTORS. Nancy S.

Foster and Carl A. Koval, University of Colorado.

3:45: SYNTHESIS OF STOICHIOMETRIC CADMIUM SELENIDE FILMS VIA

SEQUENTIAL MONOLAYER ELECTRODEPOSITION. Michael J. Sailor,

Vincent V. Doan, Jon D. Klein, and Ann M. Kressin, UCSD.

4:15: DETECTION OF HOT ELECTRONS IN A PHOTOELECTROCHEMICAL CELL.

Robert Torres and Carl A. Koval, University of Colorado.

4:45: EFFECT OF POLYMER ELECTRODE MORPHOLOGY ON PERFORMANCE OF A

LITHIUM/POLYPYRROLE BATTERY. Marjorie A. Nicholson and

Charles R. Martin, Colorado State University.

Tuesday morning, July 30, 1991

R.M. Penner, Presiding

- 8:30: DETERMINATION OF CHLORINE SPECIES IN WATER BY POTENTIOMETRIC STRIPPING USING COPPER(I). <u>Calvin O. Huber</u> and Youqin Xie, University of Wisconsin-Milwaukee.
- 9:00: ELECTROCHEMICAL STUDIES OF SODIUM AS A POSSIBLE ANODE FOR ROOM TEMPERATURE MOLTEN SALT ELECTROLYTE BATTERIES. Thomas
  L. Riechel, Jeffrey A. Boon, and John S. Wilkes, U.S. Air Force Academy.
- 9:30: REDOX INDUCED PROPERTIES OF VIOLOGEN BASED MONOLAYERS
  ATTACHED TO GOLD ELECTRODES. <u>Thomas W.Schneider</u> and Daniel
  A. Buttry, University of Wyoming.
- 10:00: TEMPLATE SYNTHESIS OF MICROTUBULE ARRAYS UTILIZING ELECTROCHEMICAL AND VACUUM DEPOSITION TECHNIQUES. <u>Charles</u>
  <u>J. Brumlik</u> and Charles R. Martin, Colorado State University.
- 10:30: BREAK
- 10:45: SURFACE ENHANCED RAMAN SCATTERING OF REDOX SURFACTANT ADSORBATES ON ELECTRODES. Xiaoyan Tang and Daniel A. Buttry, University of Wyoming.
- 11:15: COUPLED ELECTRON AND ION TRANSPORT IN A CONDUCTING POLYMER:
  MIXED CATION AND ANION TRANSPORT. Alan Kopelove and C.
  Michael Elliott, Colorado State University.
- 11:45 THE ORIGINS AND IDENTITIES OF OXYGEN IN POLYPYRROLE.

  <u>Junting Lei</u>, Wenbin Liang, and Charles R. Martin, Colorado State University.

#### Poster Presentations

THERMAL, SPECTRAL AND ELECTRONIC PROPERTIES OF PERFLUOROSULFONATE IONOMER/POLYPYRROLE COMPOSITE MEMBRANES.

<u>Daniel L. Feldheim</u>, Del R. Lawson, Edward Z. Cai, and Charles R. Martin, Colorado State University.

# SYMPOSIUM ON ENVIRONMENTAL CHEMISTRY Organized by Lynda M. Faires

Tuesday morning, July 30, 1991

#### Edward T. Furlong, Presiding

8:30: ISOLATION OF MULTIPLE CLASSES OF PESTICIDES FROM LARGER-VOLUME WATER SAMPLES USING C-18 SOLID PHASE EXTRACTION CARTRIDGES. William T. Foreman and Paul M.Gates, U.S. Geological Survey; Gregory D. Foster, George Mason University.

8:50: INFLUENCE OF NONFILTERABLE PARTICLES AND COLLOIDS IN WATER
ON THE COLLECTION EFFICIENCIES OF PESTICIDES IN C-18 SOLIDSORBENT CARTRIDGES. Gregory D. Foster and Walter L. McLeod,
George Mason University.

9:10: INVITED SPEAKER IN ENVIRONMENTAL MASS SPECTROMETRY.
SPONSORED BY FINNIGAN MAT.

DIRECT SAMPLING ION TRAP MASS SPECTROMETRY FOR ENVIRONMENTAL SAMPLING. Marcus Wise. Oak Ridge National Laboratory.

10:10: BREAK

10:40: APPLICATION OF MASS SPECTROMETRY-MASS SPECTROMETRY FOR THE RAPID ANALYSIS OF ORGANIC CONTAMINANTS IN ENVIRONMENTAL SAMPLES. Edward T. Furlong, U.S. Geological Survey.

11:00: DISTRIBUTION OF SELECTED ANTHROPOGENIC ORGANIC COMPOUNDS ON SUSPENDED SEDIMENT IN THE MISSISSIPPI RIVER. College E. Rostad and Wilfred E. Pereira, U.S. Geological Survey.

11:20: CHARACTERIZATION OF ORGANIC MATTER ASSOCIATED WITH IRON-RICH
BED SEDIMENT FROM AN ACIDIC MOUNTAIN STREAM. Kathleen S.
Smith, James F. Ranville, U.S. Geological Survey; Steven C.
Gebhard, Solar Energy Research Institute; Donald L.
Macalady, Colorado School of Mines.

11:40 TOTAL ORGANIC CARBON, A COMPARATIVE STUDY. Robert L. Spraggins, Michael T. Diesing, and Timothy J. Wilhelm, Manville Technical Center.

12:00 LUNCH

Tuesday Afternoon, July 30, 1991

Mark W. Sandstrom, Presiding

1:30: EXTRACTION AND METHOD DETECTION LIMIT ENHANCEMENT FOR AQUEOUS n-NITROSODIMETHYL AMINE. Steven E. Bonde, Jacquie A. Russell, and Harry R. Hendler, Martin Marietta Astronautics Group.

1:50: METHOD DETECTION LIMIT AND ANALYSIS OF n-NITROSODIMETHYL
AMINE IN TREATED WASTEWATER. Steve E. Bonde, <u>Jacquie A.</u>
Russell, and Harry R. Hendler, Martin Marietta Astronautics
Group; Sabrina Al-Khafaji, Denver.

2:10: FORMALDEHYDE ANALYSIS BY HPLC AS 2,4-DINITROPHENYLHYDRAZONE, II. Michael T. Diesing and Robert L. Spraggins, Manville Technical Center.

2:30: BREAK

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- 3:00: DETECTION OF HAZARDOUS CONTAMINANTS WITH RAMAN FIBER OPTIC PROBES. <u>Laura Peitersen</u>, Ken Mullen, and Keith Carron, University of Wyoming.
- 3:20 PVC DOPED FILMS OF MAGNESIUM PHTHALOCYANINE FOR CHLORINE GAS DETECTION. Todd E. Lanning and Daniel A. Buttry, University of Wyoming.
- 3:40: A BIOGENIC SOURCE OF BROMINE TO THE ARCTIC TROPOSPHERE AND ASSOCIATED SPRINGTIME SURFACE OZONE DEPLETION. Paul T. Buckley, John W. Birks, and William T. Sturges, University of Colorado.

Wednesday Morning, July 31, 1991

#### Lynda M. Faires, Presiding

- 8:15 SELECTED TRACE ELEMENTS IN CANADIAN DRINKING WATER SUPPLIES.

  <u>Jean-Charles Meranger</u>, Belinda Lo, Department of National
  Health and Welfare, Ottawa, Ontario, Canada.
- 8:35: PERFORMANCE CHARACTERISTICS OF AN ICP-MS SYSTEM DESIGNED FOR DRINKING WATER ANALYSIS. Rob Henry and Chris Tye, Fisons/VG Instruments.
- 8:55: ENVIRONMENTAL APPLICATIONS OF CHELATION CONCENTRATION-INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY. Lynda M. Faires and Charles J. Patton, U.S. Geological Survey; John M. Riviello, Dionex Corporation.
- 9:15: INVITED SPEAKER. BALANCE IN ENVIRONMENTAL MEASUREMENTS: ISSUES AND CHALLENGES ASSOCIATED WITH SAMPLING. Robert L. Siegrist, Oak Ridge National Laboratory.
- 10:15: BREAK
- 10:40: METAL ANALYSIS OF SODIUM PYROPHOSPHATE EXTRACTS BY ICP-AES.

  Kathleen C. Stewart, Paul H. Briggs, and Clara S.E. Papp,
  U.S. Geological Survey.
- 11:00: TRACE DETERMINATION AND SPECIATION OF CYANIDE BY ATOMIC ABSORPTION SPECTROSCOPY. <u>Jeffrey J. Rosentreter</u> and Rodney K. Skogerboe, Colorado State University.
- 11:20: HIGH-SPEED, SIMULTANEOUS DETERMINATION OF TOTAL KJELDAHL NITROGEN AND TOTAL PHOSPHORUS IN WATER SAMPLES. Charles J. Patton, U.S. Geological Survey.
- 11:40: ACID DIGESTION OF WATER SAMPLES USING CLOSED PLASTIC CONTAINERS AND A CONVENTIONAL LABORATORY OVEN. Gerald L.

Hoffman, Randall C. Daniel, Juliana W. Fahey, Betty J.
McLain, U.S. Geological Survey.

12:00: LUNCH

# 14TH INTERNATIONAL SYMPOSIUM ON EPR Organized by Gareth Eaton and Sandra Eaton

Monday Morning, July 29, 1991

Session I - How Good is EPR at Determining Atom Positions?

#### John Weil, Presiding

| 8:30 Opening Remarks - S.S. | Eaton |
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- 8:40 <u>KEYNOTE LECTURE</u> THE STUDY OF STRUCTURE BY ELECTRON PARAMAGNETIC RESONANCE METHODS. <u>C.A. Hutchison Jr.</u>, University of Chicago.
- 9:25 DERIVATION OF TRUE IMPURITY-LIGAND DISTANCES FROM EPR AND OPTICAL PARAMETERS. M. Moreno, University of Cantabria, Spain.
- 10:05 COFFEE BREAK
- 10:35 ENDOR DETERMINED ACTIVE SITE STRUCTURE OF TRUE ENZYME REACTION INTERMEDIATES. M.W. Makinen, D. Mustafi, G.B. Wells, and J.M. Troyer, University of Chicago.
- 11:15 <u>PLENARY LECTURE</u> DETERMINATION OF ATOMIC POSITIONS BY ENDOR OF POINT DEFECTS IN SOLIDS. <u>J.-M. Spaeth</u>, University of Paderborn, Germany.
- 12:00 LUNCH

Monday afternoon, July 29, 1991

Session II - How Good is EPR at Determining Atom Positions?

#### Michael Bowman, Presiding

- 1:30 MEMBRANE PROTEIN STRUCTURE AND TOPOLOGY BY SITE-DIRECTED SPIN LABELING. C. Altenbach, T. Marti, D.A. Greenhalgh, S. Flitsch, H.G. Khorana, and W. L. Hubbell, UCLA and MIT.
- 2:05 NOVEL EFFECTS IN PULSED ENDOR. <u>P.E. Doan</u>, C. Fan, C.E. Davoust, B.M. Hoffman, Northwestern University.
- 2:30 ELECTRON SPIN ECHO ENVELOPE MODULATION STUDIES OF Ni(III) MODEL COMPLEXES. J.-W. Hwang, H.-I. Lee and <u>J.L. McCracken</u>, Michigan State University.

| 2:55        | BREAK   |
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| 3:25        | THE GLORIES OF ESEEM: MEASURING ELECTRON-NUCLEAR DIPOLAR COUPLINGS IN ORIENTATIONALLY DISORDERED SOLIDS. $\underline{D.J.}$ Singel, Harvard University.   |
| 3:50        | PLENARY LECTURE - PROPERTIES OF BASIC AND COMBINATION FREQUENCY LINES IN ESEEM SPECTRA OF ORIENTATIONALLY DISORDERED SOLIDS. S.A. Dikanov, Institute of Chemical Kinetics and Combustion, USSR. |
| 4:20        | Open Discussion: How good is EPR at determining atom positions? Michael Bowman, Chairing.   |
| 4:45        | Business meeting of International EPR Society   |
| Tuesday mor | ning, July 30, 1991   |
| Session III | - EPR Standards, Robert Clarkson, Presiding   |
| 8:30        | QUALITY ASSURANCE IN EFR. S.S. Eaton and $\underline{G.R.}$ Eaton, University of Denver.  |
| 9:00        | EFR STANDARDS DEVELOPMENT AT NIST. $\underline{M}, F$ . Describers, National Institute of Standards and Technology.   |
| 9:30        | BREAK - be sure to see the exhibits   |
| 10:15       | USE OF STANDARD SAMPLES FOR ENDOR SPECTROSCOPY. R.A. Isaacson, University of California, San Diego.   |
| 10:45       | STANDARDS IN QUANTITATIVE EPR SPECTROSCOPY: SEARCH FOR A NEW PITCH STANDARD. <u>I. Goldberg</u> and T.M. McKinney, Rockwell International.  |
| 11:15       | DIOXYGEN GAS AS AN EFR STANDARD. S.M. Manley, J. Minga, M. Mizushima, M.J. Mombourquette, and $\underline{J.A.~Weil}$ , University of Saskatchewan.   |
| 11:35       | Open discussion of EPR standards, R. Clarkson, Chairing   |
| 12:00       | LUNCH   |
| Tuesday aft | ernoon, July 30, 1991   |
| Session IV  | - ENDOR, Harvey Buckmaster, Presiding   |

THE STRUCTURE OF CAROTENOID CATION RADICALS: AN ENDOR AND

MOLECULAR ORBITAL STUDY. L. Piekara-Sady, M. Khaled, E.

1:30

Bradford, L.D. Kispert, and M. Plato, University of Alabama and Free University Berlin.

- 1:50 ENDOR DETERMINED STRUCTURES AND CONFORMATIONS OF CHROMOPHORIC OLEFINIC DERIVATIVES OF 2,2,5,5-TETRAMETHYL-1-OXYPYRROLINYL SPIN LABELS. <u>D. Mustafi</u>, W.E. Boisvert, and M.W. Makinen, University of Chicago.
- 2:10 COHERENCE IN COUPLED ELECTRON AND NUCLEAR SPIN SYSTEMS. H. Thomann and M. Bernardo, Exxon Research Laboratory.
- 2:30 BREAK

Session V - Posters, S.S. Eaton, Presiding

- 3:00 4:00 authors present for posters labeled A 4:00 5:00 authors present for posters labeled B
- A DIELECTRIC RESONATOR FOR 9 GHz ENDOR/EPR INCORPORATING EFFICIENT LIGHT IRRADIATION. R.A. Isaacson and G. Feher, Univ. of California, San Diego.
- B LONG-RANGE COUPLING IN EPR-ENDOR OF 3-[n]STAFFYL RADICALS.

  A.J. McKinley, P. Ibrahim, P. Kaszynski, V. Balaji, and J.

  Michl, University of Texas at Austin.
- A ENDOR AND ESEEM STUDIES OF THE TRIPLET DIMER AND DOUBLET MONOMER OF BIS(PYRIDINE-2-METHANOLATO)COPPER(II). Y. Ohba, S. Kawata, M. Satoh, H. Yokoi, and M. Iwaizumi, Tohoku University, Japan.
- B EFR AND ENDOR STUDIES OF VANADYL-NUCLEOTIDE COMPLEXES. <u>D. Mustafi</u>, J. Telser, and M.W. Makinen, University of Chicago.
- A PULSED ENDOR STUDIES ON METALLOPROTEINS. C. Fan, P.E. Doan, C.E. Davoust, and B.M. Hoffman, Northwestern University.
- B Q-BAND ENDOR OF <sup>2</sup>H-, <sup>13</sup>C-, and <sup>15</sup>N-LABELLED TRP IN ES.

  <u>A.L.P. Houseman</u>, M. Sivaraja, D. Goodin, and B.M. Hoffman,
  Northwestern University.
- A HYPERFINE INTERACTION WITH  $\beta$ -FLUORINE IN NITROXIDE RADICALS. DETERMINATION OF RELATIVE ORIENTATION OF g- AND A-TENSORS FROM POWDER 2mm AND X-BAND EFR SPECTRA. V.I. Gulin, S.A. Dikanov, and Yu. D. Tsvetkov, Institute of Chemical Kinetics and Combustion, USSR.
- B MULTIFREQUENCY ESEEM IN S=5/2 SYSTEMS: STUDIES OF  $m_1^{2+}$  SUBSTITUTED N-RAS p21. R.G. Larsen and D.J. Singel, Harvard University.

- A EFFECTS OF ZERO-FIELD SPLITTING ON ESEEM OF MANGANESE. A.R.

  Coffino and J. Peisach, Albert Einstein College of Medicine.
- B PULSED ELECTRON-NUCLEAR MULTIPLE RESONANCE STUDIES OF IRON SULFUR CLUSTERS. M. Bernardo and <u>H. Thomann</u>, Exxon Research Laboratory.
- A DESIGN CONSIDERATIONS FOR BROADBAND EFR SPECTROMETER OPERATION. <u>C. Bender</u>, S.G. Gedam, and J. Peisach, Albert Einstein College of Medicine.
- B APPLICATION OF THE BLOCH EQUATIONS TO CONTINUOUS WAVE MULTI-QUANTUM ELECTRON PARAMAGNETIC RESONANCE. M. Jelen and <u>W.</u> <u>Froncisz</u>, Jagiellonian University, Poland.
- A SIMULATIONS OF THE RESONANCE LINES IN CONTINUOUS WAVE MULTI-QUANTUM ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY. W. Froncisz and M. Jelen, Jagiellonian University, Poland.
- B SATURATION RECOVERY ELECTRON PARAMAGNETIC RESONANCE SPECTROMETER. W. Froncisz, J. Koziol, J. Ilnicki, W. Galinski, and T. Oles, Jagiellonian University, Poland.
- A THE MAGNETIC AND ELECTRIC FIELD DISTRIBUTIONS IN CYLINDRICAL MULTI-GAP RESONATORS. W. Piasecki and W. Froncisz, Jagiellonian University, Poland.
- B COMPLICATIONS IN THE MEASUREMENT OF THE MAGNETIC FIELD PENETRATION DEPTH IN YBa2Cu3O $_{\rm X}$  and Bi2Sr2CaCu2O $_{\rm X}$  SUPERCONDUCTORS BY ELECTRON SPIN RESONANCE LINE BROADENING OF SURFACE PARAMAGNETIC PROBES. J.T. Masiakowski, M. Puri, and L. Kevan, University of Houston.
- A MODULATION BROADENING OF VOIGT LINES. M. Peric and H.J. Halpern, University of Chicago.
- B A METHOD TO ENHANCE THE RESOLUTION OF OVERLAPPING EPR LINES.

  A. Cabral-Prieto, H. Jimenez-Dominguez, L. Gonzales-Tovany,
  and M. Torres-Valderrama, Instituto Nacional de
  Investigaciones Nucleares, Mexico.
- A SPATIAL DISTRIBUTION OF FREE RADICAL GENERATED ON THE SURFACE OF SOLID ORGANIC MATERIAL BY GLOW DISCHARGE. V.V.

  Kurshey, T. Ichikawa, and A.M. Raitsimring, Hokkaido University and Institute of Chemical Kinetics and Combustion, USSR.
- B SATURATION RECOVERY STUDIES ON SPIN LABELS. <u>J.-J. Yin</u>, O. Grinberg, and J.S. Hyde, Medical College of Wisconsin.
- A IMPACT OF IRON(III) ON NITROXYL RELAXATION TIMES. M.H.
  Rakowsky, S.S. Eaton, and G.R. Eaton, University of Denver.

- E COMPARISON OF ELECTRON SPIN RELAXATION RATES FOR Cr(V) AND NITROXYL RADICALS. K. Nakagawa, S.S. Eaton, and G.R. Eaton, University of Denver.
- A PHOTOIONIZATION OF NEUTRAL AND POSITIVELY CHARGED ALKYLPHENOTHIAZINES IN POSITIVE, NEUTRAL, AND NEGATIVELY CHARGED VESICLES: EFFECTS OF THE ALKYL CHAIN LENGTH. P. Bratt, Y.S. Kang, and L. Kevan, University of Houston.
- B INVESTIGATION OF POLYIMIDES USING EPR SPECTROSCOPY. M.K. Ahn, T.C. Stringfellow, and K.J. Bowles, Indiana State University and NASA Lewis Research Center.
- A EFFECT OF CLOFIBRATE AND PROBUCOL ON PHASE TRANSITION AND FLUIDITY OF DIMYRISTOYLPHOSPHATIDYLCHOLINE MEMBRANES. A SPIN LABEL STUDY. A. Pezeshk, J. Wojas, and W.K. Subczynski, Moorhead State University and Jagiellonian University.
- B EFFECTS OF CHOLESTEROL, ALKYL CHAIN LENGTH AND UNSATURATION ON THE SHAPE OF THE HYDROPHOBIC BARRIER OF PHOSPHOLIPID BILAYERS. W.K Subczynski, A. Wisniewska, J.S. Hyde, and A. Kusumi, National Biomedical ESR Center, Jagiellonian University, and Tokyo University.
- A MEASUREMENTS OF PARTITION CONSTANTS OF SEMIQUINONES DISTRIBUTED BETWEEN PHOSPHATIDYLCHOLINE AND BUFFER PHASES USING THE SPIN-BROADENING TECHNIQUE. A.E. Alegria, M. Morales, and S. Rivera, University of Puerto Rico.

Wednesday morning, July 31, 1991

#### Session VI, Dale Pace, Presiding

- 8:30 250 GHz EPR STUDIES OF SOLID-STATE MATERIALS. W.B. Lynch, K.A. Earle, R.H. Crepeau, <u>D.E. Budil</u>, and J.H. Freed, Cornell University.
- 9:00 ELECTRON SPIN RESONANCE STUDY COMPARING E' TRAPPING CENTERS IN SIMOX AND THERMAL OXIDES. J.F. Conley, P.M. Lenahan, and P. Roitman, Pennsylvania State University.
- 9:20 THE REVERSIBILITY OF LIGHT-INDUCED ESR SIGNALS IN SILICON NITRIDE. M.S. Crowder, E. Sigari, E. Tober, and J. Kanicki, IBM and University of California, Davis.
- 9:45 EFR AND ODMR STUDIES OF INTERSTITIAL METAL ATOMS AND LATTICE VACANCIES IN M<sub>2</sub>P<sub>2</sub>S<sub>6</sub> SINGLE CRYSTALS. S. Sibley and A.H. Francis, University of Michigan.
- 10:10 BREAK

- 10:40 IMPLICATIONS OF HYPERFINE ANISOTROPY ON THE DETERMINATION OF 14N QUADRUPOLE AND HYPERFINE INTERACTIONS FROM MULTIFREQUENCY ELECTRON SPIN-ECHO ENVELOPE MODULATION PATTERNS. S.A. Cosgrove and D.J. Singel, Harvard University.
- 11:00 MONTE CARLO FROCEDURES FOR THE PRECISE EVALUATION OF THE SPIN HAMILTONIAN PARAMETERS FROM EPR DATA. <u>E. Laredo</u>, A. Bello, M. Diaz, N. Suarez, M. Puma, Simon Bolivar University, Venezuela.
- 11:20 A RELATIVISTIC EFFECTIVE HAMILTONIAN FOR S-STATE IONS. H.A. Buckmaster and R. Chatterjee, University of Calgary.
- 11:40 EFR OF Cu<sup>2+</sup> DOPED POTASSIUM OXALATE MONOHYDRATE: JAHN-TELLER EFFECT AND POSITIONS OF Cu<sup>2+</sup> IONS. <u>S.K. Misra</u>, X. Li, and C. Wang, Concordia University.
- 12:00 LUNCH

Wednesday afternoon, July 31, 1991

Session VII, Wolfgang Trommer, Presiding

- 1:30 VISCOSITY MEASUREMENTS IN THE PLASMA MEMBRANE OF HUMAN KERATINOCYTES BY EPR SPECTROMETRY. C.L. Marcelo, W.R. Dunham, S.B. Klein, L.M. Rhodes, and R.H. Sands, University of Michigan.
- 1:50 CONFIGURATION AND DYNAMICS OF SOLVATED, ALKYL BONDED SILICA PHASES STUDIED BY SPIN LABEL TECHNIQUES. R.G. Kooser, J. Heindl, B. Poland, and M.A. Guzeldere, Knox College.
- 2:10 MULTIFREQUENCY INVESTIGATIONS INTO THE ORIGIN OF THE S2-STATE SIGNAL AT g=4 OF THE O2-EVOLVING COMPLEX. A. Haddy, W.R. Dunham, R.H. Sands, and R. Aasa.
- 2:30 BREAK

Session VIII - Posters, S.S. Eaton, Presiding

- 3:00 4:00, authors present for posters labeled C 4:00 5:00, authors present for posters labeled D
- C A RE-INVESTIGATION OF CHROMATIUM VINOSUM HIGH-POTENTIAL IRON-SULFUR PROTEIN BY EPR AND MOSSBAUER SPECTROSCOPY. W.R. Dunham, W.R. Hagen, J.A. Fee, and R.H. Sands, University of Michigan.

- D THE IRON IN LIPOXYGENASES BY EPR AND MOSSBAUER SPECTROMETRY.

  R.H. Sands, R.T. Carroll, J.F. Thompson, W.R. Dunham, and
  M.O. Funk, Jr., University of Michigan and USDA.
- C LOW LEVEL OXIMETRY BY EFR IN VIVO: OPTIMIZATION OF SPECTROSCOPIC CONDITIONS FOR NARROW LINE STUDIES. A.I. Smirnov, T. Walczak, J. Liu, S.W. Norby, D. Brown, and H.M. Swartz, University of Illinois.
- D INTERACTION OF 3-HYDROXYBUTYRATE DEHYDROGENASE (BDH) WITH ACTIVATING LECITHINS AS STUDIED BY ESR IN ORDERED MEMBRANES.

  K.K. Klein, B. Rudy, J.O. McIntyre, S. Fleischer, and W.E.

  Trommer, University of Kaiserslautern, Germany.
- C AN EPR INVESTIGATION OF SPIN LABELLED ERYTHROCYTES FROM MALIGNANT HYPERTHERMIA SUSCEPTIBLE PATIENTS. <u>H.A.</u>
  <u>Buckmaster</u>, P. Cooper, J. Kudynska, and R. Kudynski, University of Calgary.
- D EPR OBSERVATIONS OF TEMPO QUENCHING IN MONITORING THF- $\alpha$  CYTOTOXICITY IN L929 CELLS. S. Mishra, B.R. Misra, and <u>H.P. Misra</u>, Virginia Tech.
- C SPIN TRAPPING AT 250 MHz WITH VARIABLY DEUTERATED SPIN TRAPS TO ENHANCE SENSITIVITY: THE POSSIBILITY OF IN VIVO SPIN TRAPPING. H.J. Halpern, M. Peric, E. Barth, S. Pou, and G.M. Rosen, University of Chicago and University of Maryland School of Pharmacy.
- D VISUALIZATION OF EDDY CURRENT LOSS IN L-BAND ESR IMAGING.

  T. Ogata, M. Ono, and L.J. Berliner, Yamagata University and Ohio State University.
- C HIGH FIELD EPR MICROIMAGING IN CRYOBIOLOGY INVESTIGATIONS.

  A.I. Smirnov, O.G. Poluectov, and Y.S. Lebedev, University of Illinois and Institute of Chemical Physics, Moscow.
- D DEPTH PROFILE OF E' CENTERS IN IRRADIATED SILICON DIOXIDE.
  D. Kerwin, A. Miller, M. Sueki, G.R. Eaton, S.S. Eaton, and
  F. Galeener, Colorado State University and University of Denver.
- C CONFORMATION OF A FIVE-MEMBERED RING CONTAINING A PHOSPHINYL RADICAL: AB INITIO FREDICTIONS AND ESR STUDY. M. Geoffroy and G. Terron, University of Geneva, Switzerland.
- D FREE RADICAL MECHANISMS IN HIGH DENSITY NITRO-COMPOUNDS: HEXANITROISOWURTZITANE, A NEW HIGH-ENERGY NITRAMINE. M.D. Pace, Naval Research Laboratory.

- C THE Mn<sup>2+</sup> HFS SPECTRUM IN ARGONNE COALS AT 9 AND 33 GHz. H.A. Buckmaster, J. Kudynska, and Y.P. Zhang, University of Calgary.
- D EPR STUDIES OF SPIN DYNAMIC PROPERTIES IN KONDO SYSTEM.

  N.G. Fazleev, UCLA and Kazan State University.
- C MAGNETIC RESONANCE STUDIES OF MULTIPOLAR INTERACTIONS IN METALS AND ALLOYS WITH RARE-EARTH IMPURITIES. N.G. Fazleev, UCLA and Kazan State University.
- D DIRECT EVIDENCE FOR Mm SUBSTITUTION IN A FRAMEWORK SITE IN MmAPO-11 MOLECULAR SIEVE FROM THE ADSORBED WATER COORDINATION CONFIGURATION DEDUCED BY ELECTRON SPIN ECHO MODULATION ANALYSIS. G. Brouet, X. Chen, and L. Kevan, University of Houston.
- C DETERMINATION OF DEFECT CONCENTRATIONS CO-EXISTING IN SINGLE AND DOUBLE-DOPED CaF<sub>2</sub> CRYSTALS BY EPR TECHNIQUES. A. Bello, M. Diaz, N. Suarez, and E. Laredo, Simon Bolivar University, Venezuela.
- D OPTICALLY DETECTED ENDOR OF DEFECTS IN III-V SEMICONDUCTORS.

  H.C. Crookham and T.A. Kennedy, Naval Research Laboratory.
- C PHOTOINDUCED PARAMAGNETIC CENTERS IN AMORPHOUS SILICON OXYNITRIDE. <u>J.T. Yount</u>, G.T. Kraus, P.M. Lenahan, and D.T. Krick, Pennsylvania State University and Intel Corporation.
- D EPR STUDIES OF [TiO4/Na] DEFECTS IN QUARTZ. P. Bailey and J.A. Weil, University of Saskatchewan.
- C MODIFICATION OF THE  $V_k$ -CENTER MODEL IN KCl SINGLE CRYSTALS AN EPR AND ENDOR INVESTIGATION. Y. Zhang and S.A. Marshall, Michigan Technological University.
- D AN EPR STUDY OF COLOR CENTERS IN KF DOPED WITH AgF. C. Yu and S.A. Marshall, Michigan Technological University.
- C. CARBOXYVERDAZYLS: WATERSOLUBLE FREE ORGANIC RADICALS. D. Ding, M.P. Eastman, A.J. Mayr, C. McClellan, and R. Willink, Northern Arizona University.
- D SPIN-LABELING OF METAL SITES ON THE SARCOPLASMIC RETICULUM ATPase WITH TEMPAMINE BY USING A CARBODIIMIDE AS A COUPLING AGENT. C. Coan, P. Jakobs, and A. Murphy, University of the Pacific.
- C TWO-DIMENSIONAL ORIENTATION SELECTIVE ESEEM ON DISORDERED SYSTEMS. J.J. Shane, E.J. Reijerse, E. deBoer, and P. Hofer. University of Nijmegen and Bruker.

D APPLICATION OF VERY LOW FREQUENCY EFR IMAGING TO PHANTOMS OF ALANINE DOSIMETERS. A. Sotgiu, University of l'Aquila.

Wednesday evening

Open House at the University of Denver EPR Laboratory

Thursday morning, August 1, 1991

Session VIII - Karl Hausser, Presiding

- 8:30 FROGRESS IN IN VIVO EPR SPECTROSCOPY TO MEASURE THE CONCENTRATION OF OXYGEN [Oz]. H.M. Swartz, S. Boyer, D. Brown, P. Gast, J. Glockner, H. Hu, J. Liu, M. Moussavi, S. Norby, A. Smirnov, N. Vahidi, T. Walczak, M. Wu, and R. Clarkson, University of Illinois.
- 9:05 AN ABSOLUTE OXYMETRY IN LIVING ANIMAL TISSUE. H.J. Halpern, M. Peric, and E. Barth, University of Chicago.
- 9:35 FOURIER TRANSFORM ELECTRON PARAMAGNETIC RESONANCE IMAGING.
  R.H. Crepeau, U. Ewert, C.R. Dunnam, D. Xu, S. Lee, and J.H.
  Freed, Cornell University.
- 10:05 BREAK
- 10:30 DESIGN CONSIDERATION FOR OPTIMIZING THE PERFORMANCE OF RESONANT CAVITIES FOR PULSED EFR. S.G. Gedam, C. Bender, and J. Peisach, Albert Einstein College of Medicine.
- 11:00 ELECTRONIC TUNING OF LOOP-GAP RESONATORS. G.A. Rinard, R.W. Quine, and G.R. Eaton, University of Denver.
- 11:30 TWO-DIMENSIONAL FOURIER TRANSFORM ESR STUDIES OF NUCLEAR MODULATION. B.R. Patyal, S. Lee, and <u>J.H. Freed</u>, Cornell University.
- 12:00 LUNCH

Thursday afternoon - Bruker user's meeting. Please contact Dr. Art Heiss if you wish to participate.

NOTE: Poster presenters are requested to display their posters from Monday morning to Thursday morning to permit time for browsing.

## SYMPOSIUM ON FTIR/NEAR-IR Organized by A.R. Chughtai and Joseph Montolvo

Monday, July 29, 1991

- 8:30 CATALYTIC EFFECTS OF INCORPORATED SOOTS ON WET SO2 OXIDATION. <u>Abdul R. Chughtai</u>, Michael H. Brooks, and Dwight M. Smith, University of Denver.
- 9:00 FROTEIN SECONDARY STRUCTURE FROM FOURIER TRANSFORM INFRARED SPECTROSCOPY. Ronald W. Sarver and William C. Krueger, The UpJohn Company.
- 9:30 THE APPLICATION OF INFRARED MICROSPECTROSCOPY TO PAINT CHIP ANALYSIS. <u>Ben Garland</u> and Richard T. Carl, Nicolet Spectroscopy Research Center; and J. Russell Davis, II and Sandra L. Poltorak, Tennessee Bureau of Investigation.
- 10:00 BREAK
- 10:15 NEAR-INFRARED/FT RAMAN SPECTROSCOPY. W.D. Perkins, The Perkin-Elmer Corporation.
- 10:45 RAPID IDENTIFICATION USING QUALITATIVE ALGORITHMS FOR THE NEAR-INFRARED. <u>Stephen L. Monfre</u> and Paul J. Brimmer, NIRSystems, Incorporated.
- 11:15 SIMULATING THE NIR REFLECTANCE OPTICAL PATH OF COTTONS GROUPED ACCORDING TO FIBER CROSS-SECTIONAL DIMENSIONS.

  Joseph G. Montalvo, Jr., United States Department of Agriculture.
- 11:45 EXTRACTING INFORMATION ON FIBER PROPERTIES FROM THE NIR SPECTRA OF COTTON SAMPLES. Steven M. Buco, Statistical Resources Incorporated; Joseph G. Montalvo, Jr., and Sherman Faught, United States Department of Agriculture.

# GAS, ION & SUPERCRITICAL FLUID CHROMATOGRAPHY SYMPOSIA Organized by Bill Williams

Monday, July 29, 1991

Bill Williams, Presiding

- 8:30: Introduction
- 8:45 GAS CHROMATOGRAPHIC DETERMINATION OF SODIUM MONOFLUOROACETATE AS THE FREE FATTY ACID IN AN AQUEOUS SOLVENT. Bruce A. Kimball and Elizabeth A. Mishalanie, United States Department of Agriculture.
- 9:10: COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY FOR THE SIMULTANEOUS DETERMINATION OF BOTH VOLATILITY AND POLARITY.

  Zaiyou Liu, C. J. Venkatramani and John B. Phillips, Southern Illinois University.

| 9:35                          | BREAK   |  |
|-------------------------------|---|--|
| 10:15                         | MEASUREMENT OF NITROGEN AND SULFUR SPECIES IN PETROCHEMICALS USING GAS CHROMATOGRAPHY WITH CHEMILUMINESCENCE DETECTORS.  Randy Shearer, Dee O'Neal, Ray Rios, Beth Pool and Mary David Baker. Shell Development Co.   |  |
| 10:40                         | CALCULATION OF BREAKTHROUGH VOLUMES OF IONS VIA DISTRIBUTION RATIOS IN FRONTAL ELUTION CHROMATOGRAPHY. <u>Helmut Lutsep</u> , Photo Color Systems Division, 3M Corp.  |  |
|                               | SYMPOSIUM ON LUMINESCENCE Organized by Marvin C. Goldberg   |  |
| Tuesday, July 30, 1991        |   |  |
| Marvin C. Goldberg, Presiding |   |  |
| 8:50                          | $\begin{array}{lll} \textbf{INTRODUCTORY} & \textbf{REMARKS.} & \textbf{Marvin C. Goldberg, U.S. Geological Survey.} \end{array}$   |  |
| 9:00                          | AN INTERACTION MODEL FOR SOLID-MATRIX PHOSPHORESCENCE ON FILTER PAPER VIA MODULUS AND HYDROGEN-BOND-DOMINATED MATRICES. R.J. Hurtubise and S.M. Ramasamy, University of Wyoming.                                      |  |
| 9:30                          | THE EFFECTS OF MOISTURE ON THE SOLID-MATRIX LUMINESCENCE PROPERTIES OF 4-PHENYLPHENOL ADSORBED ON FILTER PAPER. $\underline{B.B.}$ Purdy and R.J. Hurtubise, University of Wyoming.                                   |  |
| 10:00                         | BREAK   |  |
| 10:30                         | SOLID-MATRIX LUMINESCENCE PROPERTIES OF THE TETROLS OF BENZO(a)PYRENE-DNA ADDUCTS ADSORBED ON $\alpha$ -, $\beta$ -, AND $\gamma$ -CYCLODEXTRIN/NaC1 MIXTURES. J.S. Corley and R.J. Hurtubise, University of Wyoming. |  |
| 11:00                         | LUMINESCENCE CHARACTERIZATION OF ETHYLENE-VINYL ACETATE (EVA) ENCAPSULANT FOR PV MODULES.<br>F.J. Pern, Solar Energy Research Institute.  |  |
| 11:30                         | LUNCH   |  |
| 1:30                          | HYDROLOGIC APPLICATIONS OF EEM SPECTRA. Marvin C. Goldberg and Karen K. Francis, U.S. Geological Survey.  |  |
| 2:00                          | THE EFFECT OF STRUCTURE AND CONJUGATION OF ORGANIC MOLECULES  |  |

ON 3-DIMENSIONAL FLUORESCENCE SPECTRAL FEATURES. <u>Kar</u> <u>Francis</u> and Marvin C. Goldberg, U.S. Geological Survey.

- 2:30 DEVELOPMENT OF A REMOTE URANYL SENSOR BASED ON A FLOW OPTRODE. <u>Pierre Varineau</u>, Richard Duesing, and Lawrence Wangen, Los Alamos National Laboratory.
- 3:00 CONCLUDING REMARKS, Marvin C. Goldberg
- 3:05 Poster Presentation: A NEW EXPEDITIOUS APPROACH TO STUDY THE QUENCHING OF ELECTRONICALLY EXCITED URANYL ION WITH AROMATIC HYDROCARBONS AND RELATED COMPOUNDS. Mohan S. Sidhu and Arti Chopra, Nanak Dev University, India.

# SYMPOSIUM ON MASS SPECTROMETRY Organized by Joseph A. Zirrolli

#### Monday, July 29, 1991

- 9:00 TANDAM MASS SPECTROMETRY OF ANIONS DERIVED FROM LEUKOTRIENES
  AND OTHER BIOLOGICALLY ACTIVE EICOSANOIDS. Robert C.
  Murphy, National Jewish Center for Immunology and
  Respiratory Medicine.
- 9:30 QUANTITATIVE ANALYSIS OF PHOSPHOLIPID MOLECULAR SPECIES BY FAB/MS/MS. <u>Kathleen Kayganich</u> and Robert C. Murphy, National Jewish Center for Immunology and Respiratory Medicine.
- 10:00 RELATIVE MERITS OF LASER DESORPTION AND ELECTROSPRAY FOR DETERMINING MOLECULAR WEIGHTS OF PEPTIDES AND FROTEINS IN MIXTURES. Randall W. Nelson, Mark H. Allen and Marvin L. Vestal. Vestec Corporation.
- 10:30 BREAK
- 10:45 ELECTRON CAPTURE NEGATIVE ION LC/MS: MAKING THE TRANSITION FROM HPLC SEPARATION TO GC/MS IN STRUCTURAL STUDIES OF ARACHIDONATE METABOLITES. Joseph A. Zirrolli and Robert C. Murphy, National Jewish Center for Immunology and Respiratory Medicine.
- 11:15 THERMOSPRAY LC/MS ANALYSIS OF OXIDIZED AND CONJUGATED METABOLITES OF PHENOLS. Sherri Banning Turnipseed, Alban J. Allentoff, Judy L. Bolton and John A. Thompson, University of Colorado.
- 11:45 LUNCH
- 1:00 APPLICATIONS OF IN BEAM IONIZATION MASS SPECTROMETRY FOR RAPID CHARACTERIZATION OF MOLECULES OF BIOLOGICAL AND GEOLOGICAL INTEREST. <u>Edward T. Furlong</u>, U. S. Geological Survey.

1:30 TASTE AND ODOR DETERMINATIONS USING MASS SPECTROMETRY AND OTHER SPECIFIC CHROMATOGRAPHIC DETECTORS. Robert L. Spraggins and Timothy J. Wilhelm, Manville Technical Center.

#### SYMPOSIUM ON NMR

Organized by M. Ahn, R. Botto, H. Eckert, J. Garbow, B.C. Gerstein, H. Thomann, A.J. Vega and J.P. Yesinowski

#### Session I - Spin Dynamics in Complex Materials

Monday, July 29, 1991

- H. Thomann, Presiding
- 8:30 USE AND LIMITATIONS OF N-QUANTUM COHERENCE IN PROBING INTERMEDIATES IN HETEROGENEOUS CATALYSTS. S.J. Hwang, T.S. King, and B.C. Gerstein.
- 9:00 PROTON SPIN DYNAMICS OF FLUIDS IN RESTRICTED GEOMETRIES. M. Herold and H. Thomann, Exxon Corporate Research and Engineering.
- 9:30 STRUCTURAL PROPERTIES OF CERAMICS PROBED BY SPIN RELAXATION.
  D. Franke, R. Maxwell, D. Lathrop, and H. Eckert, University of California, Santa Barbara.
- 10:00 BREAK
- 10:30 SPIN DIFFUSION IN POLYMERS. <u>D. Vanderhart</u>, National Institute of Standards and Technology.
- 11:00 VARIABLE TEMPERATURE AND FIELD STRENGTH RELAXATION IN ARGONNE PREMIUM COALS. <u>Kurt Zilm</u>, Yale University.
- 11:30 MEASUREMENT OF SPIN-LATTICE RELAXATION IN COALS. R. Botto and C. Tsiao, Argonne National Laboratory.
- 12:00 LUNCH

#### Session II. Carbonaceous Materials

- R. Botto, Presiding
- 1:30 CARBON-13 CP/MAS SPECTRAL ASSIGNMENT AND EDITING WITH SEPARATED LOCAL FIELD TECHNIQUES. N. Sethi, AMOCO Corporation.
- 2:00 <sup>13</sup>C MAS-ANALYSIS OF THREE REPRESENTATIVE PREMIUM COALS. H.V. Pan and <u>Gary Maciel</u>, Colorado State University.

- 2:30 MULTINUCLEAR NMR APPROACH TO THE STUDY OF COAL FLY ASH.

  <u>D.A. Netzel</u> and F.P. Miknis, Western Research Institute.
- 3:00 BREAK
- 3:30 APPLICATION OF HIGH RESOLUTION SOLID STATE <sup>1</sup>H NMR TO COAL AND RESINITE SYSTEMS. <u>J.W. Hanna</u>, A.M. Vassallo, and M.A. Wilson, CSIRO Division of Coal and Energy Technology, Australia.
- 4:00 TRIPLE RESONANCE CP/MAS <sup>13</sup>C SPECTRA OF ORGANOFLUORIDES: FRESCIENCE OF FLUOROCOAL. E.W. Hagaman, Oak Ridge National Laboratory.
- 4:30 BUCKMINSTERFULLERENE: BOND LENGTHS, MOTION IN THE SOLID,
  AND CHEMICAL SHIFT ANISOTROPY. P. Bernier, D.S. Bethune,
  R.D. Johnson, R.D. Kendrick, G. Meijer, J.R. Salem, and <u>C.S.</u>
  Yannoni, IBM.

Tuesday, July 30, 1991

### R.W. Vaughan, Memorial Lecture

8:30 CATALYSTS, SEMICONDUCTORS, AND IONS: NEW APPROACHES TO ULTRASENSITIVE MAGNETIC RESONANCE. D.P. Weitekamp, California Institute of Technology.

#### Session III. Polymers

#### M.K. Ahn, Presiding

- 9:30 THREE-DIMENSIONAL NMR IMAGING OF POLYMERS AND POLYMER BLENDS. S.L. Dieckmann, Argonne National Laboratory.
- 10:00 NMR IMAGING OF ELASTOMER BLENDS. R.A. Komoroski and S.N. Sarkar, University of Arkansas Medical Sciences.
- 10:30 BREAK
- 11:00 SOLID STATE NMR STUDIES OF POLYURETHANE DISPERSIONS. G.R.

  Quinting, A.J. Parker, S.R. Rhodes, and A.J. Lentz, The
  Sherwin Williams Company.
- 11:30 POLYMER MISCIBILITY INVESTIGATIONS: MORPHOLOGY IN ISOTOPIC BLENDS OF POLY(VINYLETHYLENE) AND BROAD GLASS TRANSITION BEHAVIOR IN BLENDS OF POLY(ISOPRENE) AND POLY(VINYLETHYLENE) USING SOLID STATE NMR. K.J. McGrath, J.B. Miller, C.M. Roland, and A.N. Garroway, Naval Research Laboratory.
- 12:00 LUNCH

#### Session IV. Silicas and Surfaces

### H. Eckert, Presiding

- 1:30 INTERPRETATION OF THE CHEMICAL SHIFT OF XENON-129 IN ZEOLITES USING <sup>129</sup>Xe NMR. M.L. Smith, D. Corbin, and C. Dybowski, University of Delaware.
- 2:00 XENON NMR SPECTROSCOPIC INVESTIGATIONS OF ZEOLITES. M.L. Smith and <u>C.R. Dybowski</u>, University of Delaware.
- 2:30 NMR OF OPTICALLY PUMPED XENON ADSORBED ON SURFACES. D. Raftery, H. Long, L. Reven, P. Tang, T. Meersmann, J. Reimer, and A. Pines, University of California, Berkeley.
- 3:00 BREAK
- 3:30 CRYOGENIC <sup>129</sup>Xe, <sup>131</sup>Xe and <sup>1</sup>H NMR OF XENON ADSORBED ON SILICA SURFACES. APPROACHES TO LASER-POLARIZED Xe-ENHANCEMENT OF SURFACE NMR. G. Cho, L.B. Moran, and <u>J.P. Yesinowski</u>, Michigan State University.
- 4:00 <sup>29</sup>Si CP-MAS NMR EXPERIMENTS FOR MONITORING <sup>1</sup>H SPIN EXCHANGE IN SILICA GEL. I-Ssuer Chuang, C.E. Bronniman, R.C. Zeigler, and <u>G.E. Maciel</u>, Colorado State University.
- 4:30 SOLID STATE NMR ANALYSIS OF SURFACES. J.E. Roberts, M.H. Alaimo, D.M. Quai, and J.W. Larsen, Lehigh University.
- 5:00 CHARACTERIZATION OF CRISTOBALITE-RELATED SILICA STRUCTURES.

  A.J. Vega and A. Saltzberg, DuPont Central Research and Development.

#### Session V. Zeolites and Intercalates

Wednesday, July 31, 1991

- J. Garbow, Presiding
- 8:30 GUEST-HOST INTERACTIONS AND INCLUSION CHEMISTRY IN ZEOLITE-Y PROBED BY DOUBLE-ROTATION NMR. R.L. Jelinek, G.A. Ozin, and A. Pines, University of California, Berkeley.
- 9:00 PROTON NMR STUDIES OF ALUMINOSILICATES. <u>J.F. Haw</u>, J. White, L. Beck, and C. Huber, Texas A&M University.
- 9:30 COMPOSITIONAL DEPENDENCE OF <sup>29</sup>SI NMR SPECTRA OF X AND Y ZEOLITES. M.T. Melchior, D.E. Vaughan, and C.F. Pictroski, Exxon Corporation Research and Engineering.
- 10:00 BREAK

- 10:30 <sup>2</sup>H NMR INVESTIGATIONS OF ION-MOLECULE INTERACTIONS IN ACTIVATED ZEOLITE CATALYSTS. M.A. Hepp, V. Ramamurthy, D.R. Corbin, and <u>C. Dybowski</u>, University of Delaware.
- 2H NMR STUDIES OF THE DYNAMICS OF SMALL ORGANIC MOLECULES IN ZEOLITES AND INCLUSION COMPOUNDS. S. Vega, I. Kustanovich, and E. Zaborowski, Weizmann Institute of Science.
- 11:30 DYNAMICS OF DEUTERATED COUPLING AGENTS ON SILICA SURFACES.

  F.D. Blum, H.J. Kang, and J.E. Gambogi, University of Missouri, Rolla.
- 12:00 LUNCH

#### Session VI. Catalysis

- A.J. Vega, Presiding
- 1:30 THE CHEMISTRY OF Mo-SUBCARBONYLS IN Na-Y ZEOLITE. C. Tway and T. Apple, University of Nebraska, Lincoln.
- 2:00 SOLID STATE NMR STUDIES OF SMALL METAL PARTICLES IN CATALYSTS AND MATRICES. <u>K.W. Zilm</u>, O.H. Han, J. Snowel, G. Larsen, and G.L. Haller, Yale University.
- 2:30 MAGNETIC RESONANCE STUDIES OF METAL CLUSTERS IN Y ZEOLITES.

  M. Narayana and T.F. Browscombe, Shell Development Company.
- 3:00 BREAK
- 3:30 HIGH RESOLUTION <sup>13</sup>C NMR STUDIES OF CATALYTIC REACTIONS AT TEMPERATURES BETWEEN 90 AND 700 K. <u>M. Pruski</u>, D.K. Sanders, T.S. King, and B.C. Gerstein, Iowa State University.
- 4:00 NUCLEAR MAGNETIC RESONANCE STUDIES OF AMMONIA ADSORPTION ON SUPPORTED VANADIA CATALYSTS. M.S. Went and J.A. Reimer, University of California, Berkeley.
- 4:30 REACTION OF ETHYLENE WITH SUPPORTED RU; IDENTIFICATION OF THE FIRST INTERMEDIATES FORMED VIA NUCLEAR SPIN DYNAMICS.

  S.J. Hwang, T.S. King and B.C. Gerstein, Iowa State University.
- 5:00 IN SITU MAS NMR INVESTIGATIONS OF METHANOL-TO-GASOLINE CHEMISTRY ON ZEOLITE CATALYST HZSM-5. E.J. Munson and J.F. Haw, Texas A&M University.

#### Session VII. New Experimental Techniques

Thursday, August 1, 1991

J.P. Yesinowski, Presiding

| 8:30  | SYNCHRONOUS AND ASYNCHRONOUS PULSE TRAINS IN MAGIC-ANGLE SPINNING NMR. J.R. Garbow and $\underline{T}$ . Gullion, Monsanto Corporate Research and Florida State University. |
|-------|---|
| 9:00  | ROTATIONAL RESONANCE IN DIPOLAR COUPLED SPIN SYSTEMS. R.G. Griffin, Francis Bitter National Magnet Laboratory, MIT.   |
| 9:30  | PRACTICAL ASPECTS OF DOUBLE ANGLE ROTATION.   |
| 10:00 | BREAK   |
| 10:30 | ENHANCEMENT OF CROSS-POLARIZATION UNDER HIGH-SPEED MASS. $\underline{X}$ . $\underline{W}_1$ and K.W. Zilm, Yale University.  |
| 11:00 | DIAMOND ANVIL CELL NMR OF $\rm H_2$ - HIGH PRESSURE AND LOW TEMPERATURE. A. Ulug, R.E. Norberg, and M.E. Conradi, Washington University.                                    |
| 11:30 | STUDIES OF TRANSITION METAL DIHYDROGEN COMPLEXES BY SOLID STATE $^1\text{H}$ NMR. $\underline{\text{L. Wisniewski}}$ and K.W. Zilm, Yale University.                        |
| 12:00 | CONFERENCE ADJOURNED  |

#### SYMPOSIUM ON QUALITY ASSURANCE

Monday, July 29, 1991

2:00 SPECIAL SYMPOSIUM

Organized by Carol Byczek and Patricia Sulik.

A panel with varied expertise will cover several aspects of implementing Good Laboratory Practice for the Environmental Protection Agency and the Food and Drug Administration.

#### TOPICS include:

- Quality Assurance more than meets the eye.
- Application of EPA GLP to aquatic toxicology testing.
- Data validation and Analytical Laboratory Auditing.
- Comparison of EPA and FDA GLP procedures.
- Quality Assurance of Veterinary Pharmaceuticals in the Analytical Laboratory.

#### PANEL MEMBERS include:

- Carol Byczek is Quality Assurance director for Colorado Animal Research Expertises, in Fort Collins, Colorado. Her 16 years of experience includes supervision of Quality Assurance and Quality Control for Good Manufacturing Practices for veterinary pharmaceuticals, as well as Quality Assurance in Good Laboratory Practice for large animal research. She is also president of the Rocky Mountain Regional Chapter of the Society of Quality Assurance.
- Alan Kreikemeier is Quality Assurance manager for Macleod Pharmaceuticals.
- Jennette Rogers is Quality Assurance Manager for the Metpath
  Laboratories in the Rocky Mountain Region. In her 8 years
  with Metpath, she has implemented and run the Total Quality
  Management Program. She is currently responsible for the
  semi-annual Quality Assurance audits of all Metpath
  satellite laboratories, and teaches a one day seminar called
  "Quality Collage" devoted to Total Quality management.
- <u>Dan Keefe</u> is the regional Quality Assurance Officer for ENSR. He is Project Quality Assurance officer for superfund projects and National Resource damage assessment project, and has been responsible for supervising aquatic toxicology testing.

#### Organized by William J. Shampine

| Wednesday, July 31, 1991 |   |  |
|--------------------------|---|--|
| 8:25                     | Welcome and Introductory remarks  |  |
| 8:30                     | DIELECTRIC ANALYSIS OF ENERGETIC MATERIALS. <u>Albert S. Tompa</u> , Robert F. Boswell, Jim Rose, Naval Ordnance Station.   |  |
| 9:00                     | ON-LINE CHEMICAL ANALYSIS OF AQUEOUS PLUTONIUM PROCESSING UTILIZING FIBER OPTICS AND SPECTROPHOTOMETRY. Kathy M. Swan, EG & G.  |  |
| 9:30                     | CERTIFICATION OF OPTICAL TRANSMITTANCE STANDARD REFERENCE MATERIALS FOR SPECTROPHOTOMETRY. <u>Jerry D. Messman</u> , Melody V. Smith, National Institute of Standards and Technology. |  |
| 10:00                    | BREAK   |  |
| 10:30                    | THE U.S. EPA CRADAS AND THEIR EFFECT ON EPA-CERTIFIED STANDARDS. <u>David A. Agostinelli</u> , Jack K. Crissman, Jr., Janice M. Schneider, Supelco, Inc.                              |  |

- 11:00 AN EVALUATION OF A FIELD TEST KIT FOR LEAD IN DRINKING WATER INCLUDING QUALITY ASSURANCE CONSIDERATIONS. Gregory K. George, Technology Applications, Inc.; Michael R. Schock, DWRD, USEPA.
- 11:30 LUNCH
- 1:00 FROM DATA TO DECISIONS: USING THE QA/QC DATABASE. <u>Diane</u>
  Short, Diane Short & Associates.
- 1:30 QUALITY CONTROL ON ANALYSIS OF MINE DRAINAGE SAMPLES:
  COMPARISON BETWEEN TWO LABORATORIES. Thomas R. Wildeman,
  Thomas Oliver, Julia S. Reynolds, Chemistry/Geochemistry
  Dept., Colorado School of Mines; Marvin H. Frye, Gary
  Perryman, U.S. EPA, Region VIII.
- 2:00 BREAK
- 2:30 COORDINATION OF QUALITY-ASSURANCE AND QUALITY-CONTROL FROGRAMS AT THE U.S. GEOLOGICAL SURVEY'S NATIONAL WATER QUALITY LABORATORY. Thomas J. Maloney, Merle W. Shockey, Mary E. Cast, C. Ann Watterson, U.S. Geological Survey.
- 3:00 ENVIRONMENTAL PROFICIENCY TESTING IN WISCONSIN. George T.

  Bowman, William C. Sonzogni, Christopher McSweeney, Douglas
  L. Van Horn, University of Wisconsin.
- 3:30 CLOSING REMARKS

## GENERAL POSTERS Organized by Elizabeth Sexton

Posters will be set up on Monday morning through Wednesday afternoon. Authors will be available Monday afternoon between 2:00 p.m. and 4:00 p.m.

ESTIMATION OF ATMOSPHERIC PHOTOCHEMISTRY FOR ATRAZINE, SIMAZINE, ALACHLOR, AND METOLACHLOR 1. GAS PHASE PHOTOLYSIS, <u>Paul M. Gates</u>, William T. Foreman, and Wallace G. DeGiacomo. U.S. Geological Survey; Larry G. Anderson, University of Colorado at Denver.

COMPARISON OF HPLC METHOD TO THE OFFICIAL AOAC MICROBIOLOGICAL METHOD FOR DETERMINATION OF CHLORTETRACYCLINE (CTC) IN FEED. David C. Holland, Fred L. Bond, Robert K. Munns, Jose E. Roybal, Jeffrey A. Hurlbut, and Austin R. Long. Food and Drug Administration.

DETECTION OF A METHYLENE BLUE METABOLITE, THIONIN, IN MILK BYLC/VIS. <u>Jose E. Roybal</u>, Robert K. Munns, David C. Holland, Jeffrey A. Hurlbut, and Austin R. Long. Food and Drug Administration.

QUANTITATIVE MEASUREMENTS FROM VERY LOW ABSORBANCE DATA USING A FIBER OPTIC SPECTROPHOTOMETER. <u>Trevor R. Griffiths</u> and Nicolas J.Phillips\*, United States Air Force Academy, \*Present address, University of Leeds.

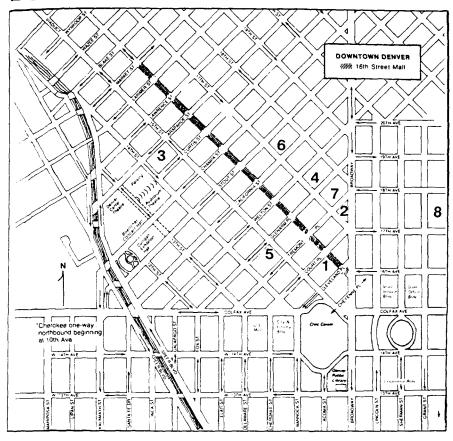
SPECTROPHOTOMETRIC DETERMINATION OF HYDROGEN PEROXIDE IN THE PRESENCE OF FLUORIDE. <u>Joseph R. Delmastro</u>, Westinghouse Idaho Nuclear Company.

DIELECTRIC ANALYSIS OF ENERGETIC MATERIALS. <u>Albert S. Tompa</u>, Robert F. Boswell, and Jim Rose, Naval Ordinance Station.

HPLC AND GC-MS DETECTION OF ORGANICS RESULTING FROM DECOMPOSITION OF HEMA (HYDROXYETHYL METHACRYLATE POLYMER) STATIONARY PHASES. <u>Jeffrey A. Hurlbut</u>, Metropolitan State College of Denver.

STRUCTURAL AND KINETIC CHARACTERIZATION OF VANADATE DERIVED AMINO ACID COMPLEXES BY 1H, 13C AND 51V NMR. Paul K. Shin and Debbie C. Crans, Colorado State University.

### **DOWNTOWN DENVER**



### Map Legend

- 1 Radisson Hotel Denver
- 2 Brown Palace Hotel
- 3 Executive Tower Inn
- 4 Hyatt Hotel
- 5 Holiday Inn-Downtown
- 6 Marriott City Center
- 7 Comfort Inn
- 8 Warwick

et al.: 33rd RMCAS Program and Registration Information

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