# **Rocky Mountain Conference on Magnetic Resonance**

Volume 39 *39th Rocky Mountain Conference on Analytical Chemistry* 

Article 1

8-3-1997

# 39th Rocky Mountain Conference on Analytical Chemistry

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# 39th Rocky Mountain Conference on Analytical Chemistry

# Abstract

Preliminary program and registration information for the 39th annual meeting of the Rocky Mountain Conference on Analytical Chemistry, co-sponsored by the Colorado Section of the American Chemical Society and the Rocky Mountain Section of the Society for Applied Spectroscopy. Held in Denver, Colorado, August 3-7, 1997.

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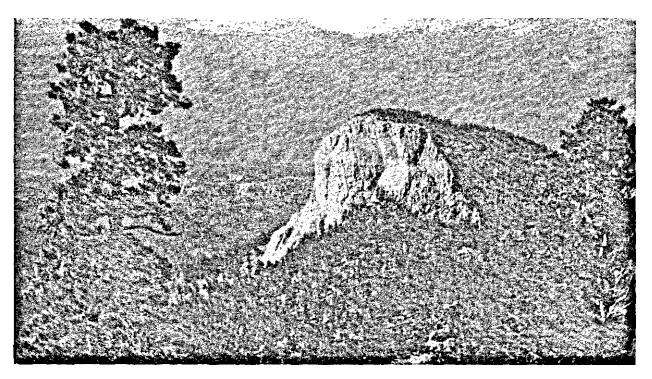


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## **Publication Statement**

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# TH ROCKY MOUNTAIN CONFERENCE ON ANALYTICAL CHEMISTRY



# PRELIMINARY PROGRAM AND REGISTRATION INFORMATION

# AUGUST 3-7, 1997

# HYATT REGENCY DENVER 1750 WELTON STREET DENVER, COLORADO

**SPONSORED BY:** 

ROCKY MOUNTAIN SECTION SOCIETY FOR APPLIED SPECTROSCOPY & COLORADO SECTION AMERICAN CHEMICAL SOCIETY

SYMPOSIA SCHEDULE								
		4/97 NDAY		5/97 SDAY		6/97 NESDAY		7/97 RSDAY
	AM	PM	AM	PM	AM	PM	AM	PM
ATOMIC/ICP-MS SPECTROSC.			X	X				
COMPOSTING		Χ						
ELECTROCHEMISTRY	X	Χ						
ENVIRONMENTAL CHEM.	X	Χ	X					
EPR	X	Х	X	X	X	X	X	
FTIR/NIR/RAMAN	X	X	X					
GENERAL POSTERS		Х						
LUMINESCENCE	X	X						
MASS SPECTROMETRY				X				
NMR	X	X	X	X	X	X	X	
PHARMACEUTICAL ANAL.			X		X	X		
RADIOCHEMISTRY	X	Х						
QUALITY ASSURANCE				X				

#### SYMPOSIA SCHEDULE

## SHORT COURSE SCHEDULE

	Wednesday 8/6/97		Thursday 8/7/97	
	AM	PM	AM	PM
ENVIROMENTAL SAMPLING	X	Χ		
COMPUTER OPERATIONS			X	Х

# VENDOR WORKSHOP SCHEDULE

	Sunday	Sunday 8/3/97 Wednesday 8/6/97		ay 8/6/97	Thursday 8/7/97		
	AM	PM	AM	PM	AM	PM	
BRUKER	X	Х				Χ	
VARIAN	X	X					
WATERS				Χ			
DIONEX			Χ	Χ			
THERMO JARRELL ASH					X		

# **UPCOMING CONFERENCE DATES**

July 25- August 1,1998 Hyatt F August 1-5, 1999 Hyatt F

Hyatt Regency Denver Hyatt Regency Denver

# **CONFERENCE LOCATION**

Technical sessions and the exhibition for the 39th Rocky Mountain Conference on Analytical Chemistry will be held in the Hyatt Regency Denver Hotel, 1750 Welton Street, Denver, Colorado 80202.

#### SYMPOSIA ORGANIZERS

#### ATOMIC SPECTROSCOPY

Gary Rayson New Mexico State University Department of Chemistry Las Cruces, NM 88003 (505) 646-5839 fax: (505) 646-2649

#### RADIOCHEMISTRY

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#### ELECTROCHEMISTRY

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#### ENVIRONMENTAL CHEMISTRY

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#### LUMINESCENCE

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Robert Hurtubise University of Wyoming Department of Chemistry Box 3838 University Station Laramie, WY 82071 (307) 766-6241 fax: (307) 766-2807

#### COMPOSTING

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#### MASS SPECTROMETRY

Joseph Zirrolli Hauser Laboratories 5555 Airport Road Boulder CO 80301 (303) 443-4662 fax (303) 441 -5803

#### NMR

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#### PHARMACEUTICAL ANALYSIS

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Patricia Sulik Rocky Mountain Instrumental Labs 456 South Link Lane Ft. Collins, CO 80524 (303) 530-1169 fax: (303) 530-1169

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Sandra Eaton University of Denver Department of Chemistry Denver, CO 80208 (303) 871 -3102 fax: (303) 871 -2254

#### FTIR/NIR/RAMAN

SPECTROSCOPY Abdul Chughtai University of Denver Department of Chemistry Denver, CO 80208 (303) 871-4404 fax: (303) 871-2932

Dwight Smith University of Denver Department of Chemistry Denver, CO 80208 (303) 871 -2938 fax: (303) 871 -2932

#### **GENERAL POSTERS**

Mary Cast National Water Quality Lab U.S.G.S. 5293 Ward Road Arvada, CO 80002 (303) 467-8135 fax: (303) 431-8331

#### ICP-MS

Howard Taylor USGS 3215 Marine Street Boulder, CO 80303 (303)541-3007 fax:(303)447-2505

#### QUALITY ASSURANCE Carl Craig Sievers Instruments 6185 Arapahoe St.

Boulder, CO 80303 (303) 444-2009 fax: (303) 444-9543

## ORGANIZERS OF THE 39TH ROCKY MOUNTAIN CONFERENCE

**CONFERENCE CHAIRMAN** 

Glenda Brown U.S. Geological Survey National Water Quality Laboratory 5293 Ward Road Arvada, CO 80002 (303) 467-8122 fax (303)431-8331

#### EXHIBITS AND VENDOR WORKSHOPS Sue Zeller Huffman Laboratories, Inc. 4630 Indiana St. Golden, CO 80403 (303) 278-4455 fax: (303) 278-7012

PUBLICITY Pat Sulik Rocky Mountain Instrumental Labs 456 S. Link Lane Ft. Collins, CO 80524 (303) 530-1169 fax: (303) 530-1169

#### **PROGRAM CHAIRMAN**

Steven Hughes Technology Experts, LLC 4450 Arapahoe St. Suite 100 Boulder, CO 80303 (303)415-2073 fax (303)415-2500

#### TREASURER

Carol Gies 14723 Mariposa Ct. Broomfield, CO 80020 (303) 277-2931

#### AUDIO-VISUAL

Colleen Gupta U.S. Geological Survey National Water Quality Laboratory 5293 Ward Road. Arvada, CO 80002 (303) 467-8147 fax: (303) 431-8331

#### REGISTRATION

Barb Coles Hauser Laboratories 5555 Airport Rd. Boulder, CO 80301 (303) 443-4662 x 1090 fax(303)441-5803

#### SOCIAL EVENTS

Donn Johnson Hauser Laboratories 5555 Airport Rd. Boulder, CO 80301 (303) 443-4662 x1077 fax(303) 441 -5803

# REGISTRATION

Admission to all technical sessions, vendor sponsored users groups and the exhibition is by the name badge for the 39th Rocky Mountain Conference. Pre-registration, using the form at the back of this program, is encouraged. The deadline for the receipt of the pre-registration form and full remittance of the conference fees is July 1, 1997. Conference fees are payable by check (denominated in \$US, only drawn on a U.S. Bank) made payable to the Rocky Mountain Conference. Visa and Mastercard are accepted, as well.

## **REGISTRATION FEES -1997**

	Preregistration	On Site
Regular (entire conference and exhibition)	\$90.00	\$110.00
One Day (specify day: M, T, W, R) includes exhibition	\$50.00	\$ 60.00
Retired / Unemployed	\$30.00	\$ 40.00
Full Time Student - Regular (includes exhibition)*	\$30.00	\$ 40.00
Student - One Day (specify day: M, T, W, R) includes exhibition*	\$20.00	\$ 25.00
Additional Vendor (beyond 3)	\$45.00	\$45.00
Exhibition Only (non-vendor)	\$15.00	\$ 15.00
Black Hawk Social Event	\$5.00	\$5.00
Environmental Sampling Short Course	\$150.00	\$175.00
Basic Computer Operations and Management	\$150.00	\$175.00

\*Legible copy of student ID must accompany registration form.

REFUNDS: Requests for refunds of conference fees must be received by July 15, 1997.

## **REGISTRATION TIMES**

On-site registration for the 39th Rocky Mountain Conference will be held in the Imperial Ballroom Foyer of the Hyatt Regency Denver during the following hours:

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Sunday, August 3	4:00 p m 8:00 p.m.
Monday, August 4	7:30 a m 3:30 p.m.
Tuesday, August 5	7:30 a m 3:30 p.m.
Wednesday, August 6	7:30 a m3:30 p.m.
Thursday, August 7	8:00 a m12:00 p.m

#### **ROCKY MOUNTAIN CONFERENCE INFORMATION**

(303) 843-9174 PO Box 506 Wheat Ridge, Colorado 80034 email: barb.coles@hauser.com

#### **ACCOMMODATION FOR DISABILITIES**

If you have a disability and may require accommodations in order to fully participate in this activity, please contact Glenda Brown (303-467-8122). We ask your cooperation in notifying us as soon as possible of your need for accommodation. While every effort will be made to meet attendees' needs, we cannot guarantee the availability of accommodations in response to requests received after July 15, 1997.

#### SOCIAL PROGRAM AT THE HYATT REGENCY DENVER

#### SCHEDULE OF EVENTS

Sunday, August 3	Registration Mixer	4:00 p.m 8:00 p.m.
Monday, August 4	Exhibition	10:00 a.m 5:00 p.m.
Monday, August 4	General Posters	3:00 p.m 5:00 p.m.
Monday, August 4	Conference Reception	5:00 p.m 7:00 p.m.
Tuesday, August 5	Exhibition	9:00 a.m 5:00 p.m.
Tuesday, August 5	Black Hawk Excursion	6:00 p.m11:30 p.m.
Wednesday, August	Exhibition	9:00 a.m 2:00 p.m.

#### **REGISTRATION NIGHT MIXER**

A cash bar will be open in the Imperial Ballroom Foyer of the Hyatt Regency Denver on Sunday evening, August 3, from 4:00 - 8:00 p.m. Plan to meet other conference attendees and beat the Monday rush to pick up your conference badge and final program.

#### **CONFERENCE RECEPTION**

On Monday evening, August 4, from 5:00 to 7:00 p.m., all attendees are cordially invited to join us for cocktails and hors d'oeuvres at the Hyatt Regency in the Imperial Ballroom. The exhibition will be open this evening and submissions from the General Poster session will be available for viewing. Enjoy music performed by last year's favorite, *Blue Heaven.* 

#### **BLACK HAWK EXCURSION**

Head for the hills on Tuesday night! Join your friends in an evening excursion to the restored mining towns of Black Hawk and Central City. Buses will be provided from the Hyatt Regency Hotel, departing at 6:00 p.m., and returning at about 12:00 midnight. Enjoy your evening in these revitalized mining towns. Your \$5.00 includes transportation each way and a discount on your dinner.

#### DIRECTIONS FROM DIA TO DOWNTOWN

Transportation is available from Denver International Airport (DIA) via bus, taxi, and private shuttle services, if you are driving, take Pena Boulevard to 1-70 westbound. Follow i-70, then exit onto 1-25 southbound. The 20<sup>th</sup> St. exit from 1-25 will take you into downtown Denver, past Coors Field. The Hyatt Regency Hotel is located at 17<sup>th</sup> and Welton Streets in downtown.

#### HOTEL ACCOMMODATIONS

Hotel rooms at the Hyatt Regency Denver, 1750 Welton Street, Denver, Colorado 80202, (303) 295-1234, are available at the **special discounted conference rate of \$110 per night (single or double), plus applicable tax.** Please identify yourself as a Rocky Mountain Conference attendee when making reservations to receive this discounted rate. Please see the Hyatt hotel reservation form in the back of this program for more information. Return this form directly to the hotel. The conference and associated social functions for the conference will be held at the Hyatt Regency Denver.

Reservations must be received by the hotel prior to **July 11,1997** and before the group reservations block is filled to assure your room accommodations. Reservations requested beyond the cut off date are subject to availability. Rooms may still be available after the cutoff date but not necessarily at the above rate. All reservations are subject to appropriate state, local, and room tax.

#### VISITOR INFORMATION

Contact the Guest Services in the main lobby of the Hyatt Regency Denver for suggestions about the large number of activities that are available in Denver and the surrounding area. For information about statewide attractions contact the Colorado Tourism Board, 1625 Broadway, Suite 1700, Denver, CO 80202, (303) 592-5510.

#### MESSAGE CENTER

Incoming telephone messages for conferees will be posted on the Conference Message Board, near the conference registration booth. The telephone numbers (303) 295-1234. Indicate that the individual is attending the Rocky Mountain Conference so the message can be posted in the proper area.

#### RESTAURANT SERVICE

The Hyatt Regency Denver has an excellent restaurant in the hotel. In addition, Guest Services in the main lobby has sample menus and suggestions for casual to elegant dining experiences throughout the Denver area.

#### JOIN THE ROCKY MOUNTAIN CONFERENCE

The Rocky Mountain Conference Organizing Committee is looking for volunteers! We are looking for additional Symposium Chairpersons and organizing committee staff. Money is available to support new symposia for start-up costs. Please contact Glenda Brown (303) 467-8122 or Steven Hughes (303) 415-2073 if you are interested in helping make a great conference even better.

#### SHORT COURSES

(Sponsored by the 39th Rocky Mountain Conference)

#### **Environmental Sampling to Meet Regulatory Compliance**

August 6, 1997

Fee: \$150preregistration \$175 on-site Faculty: John R. Dick and Steven K. Hughes

The course presents sample management techniques for environmental and /or regulatory compliance sampling. The exploration of this topic shows six major areas to be discussed. In Project Planning: Sample and Analysis plans DQO Development, Lab Selection, Laboratory Contracting, and Costs will be investigated. The pros and cons of field sampling by the client or a subcontractor will come to light in Sample Collection. In Laboratory Analysis the importance of Audits, Standard Operating Procedures and Method Selection will be shown. The pitfalls in Sample Transportation will cover: RAD Screening On-site, Packaging, Shipping, Return of Unused Samples, and Lab-Generated Waste. The section on Receipt of Analytical Data will guide you step by step through Data Verification, Data Validation and Data Quality Assessment. The final section on Record Management and Reporting demonstrates *"the job is not complete until the paperwork is done."* The overall philosophy of the course is to allow you to control quality and spend the least amount of time and money on your sampling and analysis.

#### **Basic Computer Operations and Management**

August 7, 1997

Fee: \$150preregistration \$175 on-site Faculty: Steven K Hughes and Richard Archambeau

Alternate course title: What to do until the computer repair person arrives!! This course addresses the importance of understanding the hardware in your computer. Beginning with a fundamental discussion of the functions and practices that are essential to the operation of your computer, the course will expand to cover items such as basic hardware, internal architecture, trouble shooting, minor repairs, parts replacement, and system upgrades. An in-depth description covering the importance of regular backups and how to make this as painless as possible is presented. Attendees will learn how to develop better computer practices essential to improved performance.

#### For short course information contact:

John R. Dick, PhD Technology Experts. LLC 4450 Arapahoe Ave Suite 100 Boulder, CO 80301 Tel: (303) 415-2073 Fax: (303) 415-2500 Steven K. Hughes, PhD Technology Experts. LLC 4450 Arapahoe Ave Suite 100 Boulder, CO 80301 Tel: (303) 415-2073 FAX: (303) 415-2500

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Rocky Mountain Conference on Magnetic Resonance, Vol. 39 [1997], Art. 1 EXHIBITORS FOR THE 1997 ROCKY MOUNTAIN CONFERENCE

> Exhibit Hours: Monday 10:00 a.m. to 5:00 p.m. Tuesday 9:00 a.m. to 5:00 p.m. Wednesday 9:00 a.m. to 2:00 p.m.

The following exhibitors will be in attendance, (as of May 1,1997)

Allen Scientific Glass, Inc. Analytical Instrument Recycle, Inc. American Chemical Society, Colorado Section Bruker Instruments, Inc. Chemcheck Inc. Doty Scientific, Inc. High Purity Standards JEOL USA, Inc. Nicolet Instrument Corporation Millipore Corporation Otsuka Electronics USA. Inc. Oxford Instruments. Inc. Oxford Nuclear Measurements Division Perkin-Elmer Corporation Questran Corporation Resonance Technologies, Inc. Society of Applied Spectroscopy, Colorado Section Tecmag, Inc. Thermo Jarrell Ash Update Instrument, Inc. VG Elemental Varian Associates. Inc. Waters Corporation Wilmad Glass Whatman, Inc.

# **VENDOR WORKSHOPS**

## Bruker Instruments, Inc. Sixth Annual Rocky Mountain Conference Workshop on Solid State NMR

Bruker Instruments will host a workshop dedicated to solid state NMR on Sunday, August 3, 1997 at the Hyatt Regency Hotel. New developments and products from Bruker will be presented, along with experimental results presented by users of Bruker instrumentation. All NMR spectroscopists with an interest in solids are encouraged to attend, regardless of whether they are familiar with Bruker Instruments or not. This should be an excellent opportunity to find out more about the current capabilities and future directions of Bruker in solids, and also for you to share your ideas on what you would like to see us offer in the future.

If you plan to attend, or would like more information, please contact Doug Burum at (508) 667-9580 ext. 120.

# Varian Associates Varian NMR Instruments 6th Solid State Users Conference

Varian Solids Systems' Users are invited to a users' conference on Sunday, August 3, 1997. The conference program will consist of presentations from both Varian personnel and Varian spectrometer users. Varian

applications scientists, R&D engineers, and sales representatives will be present at this half day conference. This is an excellent opportunity for long-time Varian customers to gather for an afternoon of stimulating scientific interaction, which will then adjourn for an evening of dining as guests of Varian.

For registration material please call Ms. Bee Sehrt in Palo Alto, CA at (415) 424-4526. Please indicate if you wish to make a presentation. For other information regarding this conference please contact lain Green at (314) 726-5862.

# Waters Chromatography LC/MS Seminar

Waters Corporation will present a seminar on the benefits and uses of liquid chromatography / mass spectrometry analysis. The seminar will focus on the fundamentals of such techniques as electrospray, atmospheric pressure chemical ionization (APcI), and electron impact (EI).

The advantages and range of use of each technique will be explored. This seminar will be valuable to the chromatographer currently using LC/MS, or, to the chromatographer considering adding LC/MS to the lab.

This seminar will be held Wednesday afternoon, August 6, 1997 from 1 to 4 p.m. To make reservations, contact Denise Kent at (800) 252-4752 ext. 6987.

# Dionex Corporation Industrial Applications of Ion Chromatography Accelerated Solvent Extraction (ASE)

Free Seminar and Training Workshop Wednesday, August 1997 9:00 a.m. -4:00 p.m.

Learn about the latest applications in Ion Chromatography for:

- Chemicals and Petrochemicals (brines, acids, bases, salts, amines, metals)
- Electronics and Device Extracts (ionic contamination, solvents, chemicals)
- Plating (brighteners, levelers, additives)
- Process Monitoring
- Dealing with Complex Matrices
- Trace level analysis

Learn about the recent additions to the Accelerated Solvent Extractor (ASE) and the newest industrial and environmental applications for ASE.

After lunch, (provided) attend a training workshop on:

- Pumps
- Conductivity Detectors
- Columns and Suppressors

To register, contact Lee Ramirez at (303) 771-2129 or fax your name, company, address and phone number to (303) 771-0840.

# Thermo Jarrell Ash Corporation What's New and Exciting with TJA?!!

This half day seminar is entitled "What's new and exciting with TJA?!!!" Software... Hardware...Allware!! All AA and ICP users are welcome to attend this morning session. The seminar is free and includes lunch. See you there!

To make reservations, please contact David Anderson at (303) 690-4366 or FAX at (303) 690-5934 or E-Mail at danderson@Thermo-optek.com.

# Rocky Mountain Conference on Magnetic Resonance, Vol. 39 [1997], Art. 1 A Division of Otsuka Electronics USA Inc.

8th Annual Solid-State NMR Spectroscopy Workshop

Dates: Friday, August 8th and Saturday, August 9th

Locations: Thursday evening until Saturday morning: The Elkhorn Lodge, Estes Park, Colorado

> Saturday: Otsuka Electronics USA Inc. Factory 2607 Midpoint Drive, Ste. A Fort Collins, Colorado

This will be an informal workshop in a beautiful mountain setting. Friday includes a number of speakers, informal discussions, a mixer and dinner at the Elkhorn Lodge. Saturday will include a day of lab work on various solids NMR techniques at the Otsuka Electronics headquarters in Fort Collins. Transportation from Denver to Estes Park, and to Fort Collins from Estes Park will be provided by Otsuka. There is no fee to attend the workshops, however local accommodations and meals are the attendee's expense. Space is limited, so please respond as soon as possible.

For further information contact:	Dr. Jim Frye	Tel:	970-484-0428
		Fax:	970-484-0487
		email:	jimf@chemagnetics.com

To register:

On-line registration: www.chemagnetics.com

Or

Complete the form below and return it to the following address prior to Friday, July 11th:

Pam Jarrett 2607 Midpoint Drive, Ste. A Fort Collins, CO 80525

Or, respond by email to: pjarrett@chemagnetics.com (Please include name, organization, address, telephone, fax and email address)

Date:

Please register me for this summer's Advanced Solid-State NMR Workshop: Name:

Phone:

FAX:

Organization:

Address:

#### et al.: 39th RMCAC Preliminary Program and Registration Information 39TH ROCKY MOUNTAIN CONFERENCE ON ANALYTICAL CHEMISTRY

# **TECHNICAL PROGRAM**

# PROFESSOR R.K. SKOGERBOE HONORARY SYMPOSIUM ON ATOMIC AND INORGANIC-MASS SPECTROMETRY

Organized by Howard E. Taylor and Gary Rayson

#### Tuesday, August 5,1997

Session I, Howard E. Taylor, Presiding

- 9.00 Introduction, H.E. Taylor
- 9:10 Remarks, R.K. Skogerboe
- 9:20 ANALYSIS OF ENVIRONMENTAL MATERIALS BY ICP-MS, <u>H.E. Taylor</u>, R.A. Antweiler, T.I. Brinton, D.B. Peart, D.A. Roth, U.S. Geological Survey, Boulder, CO.
- 9:45 ANALYSIS OF ROCKS BY ICP-MS, <u>F.E. Lichte</u> and A.L. Meier, U.S. Geological Survey, Denver, CO.
   10.10 THE INTERNAL STANDARD METHOD FOR ICP-MS CALIBRATION, G.W. Johnson, Matheson Gas Products, Longmont, CO.
- 10:35 Break
- 11:00 USE OF ISOTOPE DILUTION INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY TO DETERMINE MERCURY IN ENVIRONMENTAL SAMPLES, D.A. Roth and H.E. Taylor, U.S. Geological Survey, Boulder, CO.
- 11:25 HIGH-PRECISION <sup>214</sup> U/<sup>8</sup>U DISEQUILIBRIUM MEASUREMENTS IN NATURAL WATERS AND CARBONATES BY ICP-MS, <u>M.E. Ketterer</u>, C.J. Khourey and G. Matisoff, John Carroll University, University Heights, OH.
- 11:50 A REEVALUATION AND EXTENSION OF THE SCOPE OF ELEMENTS IN U.S. GEOLOGICAL SURVEY STANDARD REFERENCE WA TER SAMPLES USING ICP-MS AND ICP-AES, R.A. Antweiler, H.E. Taylor, D.A. Roth, T.I. Brinton and D.B. Peart, U.S. Geological Survey, Boulder, CO.
- 12 15 **PICOGRAM/L AND SUBPICOGRAM/L DETECTION LIMITS FOR ACTINIDES WITH ICP-MS,** <u>M.K.</u> Donais, S. Nelms, P. Shaw, J. Godfrey and F. Keenan, VG Elemental, Franklin, MA.
- Session II, Gary Rayson, Presiding
- 1:45 A NEW LOOK AT DIRECT CURRENT PLASMA SPECTROMETRY, G.N. Coleman. D. Miller and R. Starek, Thermo-Jarrell Ash, Franklin, MA.
- 2:10 A NEW CELL DESIGN FOR A RADIO FREQUENCY GLOWDISCHARGE ION SOURCE FOR GC/MS, M Belkin and J. A. Caruso, University of Cincinnati, Cincinnati, OH.
- 2:35 COMPARISON OF AXIAL VERSUS RADIAL INDUCTIVELY COUPLED PLASMA ANALYSIS, M. Cole. Varian, Sugarland, TX.
- 3.00 SPATIALLYAND TEMPORALLY RESOLVED SPECTRA OF SINGLE SHOT LASER INDUCED

PLASMAS, I. Schechter, Technion-Israel Institute of Technology, Haifa, Israel.

- 3:25 Break
- 4:00 DIRECT ELEMENTAL ANALYSIS OF INORGANIC NANOCL USTERS IN ORGANIC SOL VENTS USING GRAPHITE FURNACEAA, J.P. Wilcoxon. B. Hance, D. Stall and W. Chambers, Sandia National Laboratories, Albuquerque, NM.
- 4:25 ATOMIC ABSORPTION IN AN INDUCTIVELY COUPLED PLASMA USING AN OPTICAL SPATIAL IMAGE DISPERSION SYSTEM: ANALYTICAL FIGURES OF MERIT, G.D. Rayson and C.E. Hensman, New Mexico State University, Las Cruces, NM.
- 4:50 **INNOVATIONS IN FLAME ATOMIC ABSORPTION SPECTROMETRY, <u>D. Shrader</u>. J. Sanders, J. Moffett and B. Frary, Varian, Chicago, IL.**
- 5:15 COMPUTER SIMULATIONS OF GAS PHASE SPECIES WITHIN A GRAPHITE FURNACE ATOMIZER: IMPACT OF MATRIX COMPOSITION. G.D. Rayson and K. Sae-tueng, New Mexico State University, Las Cruces, NM.

# SYMPOSIUM ON COMPOSTING AND SUSTAINABLE AGRICULTURE

Organized by Cal Kuska and Robert L. Wershaw Composting Papers Have Been Included In The General Poster Session

# Rocky Moustin Fostiome on Menetic Prochem 578 (1997], Art. 1

Organized by Carl A. Koval

## Monday, August 4,1997

#### Morning Session

- 8.30 EFFECT OF ELECTROLYTE COMPOSITION ON ELECTRON TRANSFER KINETICS FOR FE(CN),-<sup>344</sup> AT DIAMOND-COATED GLASSY CARBON AND GRAPHITE. Qingyun Chen. Greg M. Swain, Utah State University, Logan, UT.
- 8:55 *ELECTROCHEMISTRY AT NANOELECTRODE ENSEMBLES*, <u>Michelle L. Jacobson</u>, Vinod P. Venon, Charles R. Martin, Colorado State University, Fort Collins, CO.
- 9:20 CHARGE TRANSFER KINETICS OF AQUEOUS AND ORGANIC REDOX ANALYTES AT CONDUCTIVE DIAMOND THIN FILMS, Michael C. Granger. Greg M. Swain, Utah State University, Logan, UT.
- 9:45 FURTHER INVESTIGATION OF THE REDUCTION OF ALKYL BROMIDES AT P-INP PHOTOCATHODES. HOT OR THERMALIZED ELECTRONS?, Markus D. Groner, David K Watts, Carl A. Koval, University of Colorado, Boulder, CO.
- 10:10 Break
- 10:30 IMPEDANCE-BASED SOLUTION AND VAPOR PHASE SENSING BY THIN FILMS OF POLY(3,4-DIPHENYLPYRROLE), Corey A. Salzer, C.Michael Elliott, Colorado State University, Fort Collins, CO.
- 10:55 AN ELECTROCHEMICAL ASSAY FOR DISSOLVED AZIDE USING BORON-DOPED DIAMOND ELECTRODES, Jishou Xu, Greg M. Swain, Utah State University, Logan, UT.
- 11:20 HUMIDITY-INDEPENDENT AMPEROMETRIC SENSOR FOR CARBON MONOXIDE BASED ON SOL-GEL CHEMISTRY, Mark E. Tess, James A. Cox, Miami University, Oxford, OH.

#### Afternoon Session

- 1:30
   ELECTROCHEMICALLY MODULATED COMPLEXATION FOR THE SEPARATION OF GASES, Heather

   C. Oswald, Carl A. Koval, Richard D. Noble, University of Colorado, Boulder, CO.
- 1:55 DEPOSITION AND REDOX CYCLING OF NI(OH), FILMS DEPOSITED ON BORON-DOPED DIAMOND THIN FILM ELECTRODES, Tedd E. Lister. Greg M. Swain, Utah State University, Logan, UT.
- 2:20 A CYCLIC VOLTAMMETRIC STUDY OF THE RATE CAPABILITY OF NANOFIBROUS V,O, LITHIUM-ION BATTERY ELECTRODES, Charles J. Patrissi. Charles R. Martin, Colorado State University, Fort Collins, CO.
- 2:45 ELECTROCHEMICAL INVESTIGATION OF SMALL BIOMOLECULES ENCAPSULATED BY SOL-GEL CHEMISTRY, James B. Laughlin, James A. Cox, Miami University of Ohio, Oxford, OH.
- 3:10 Break
- 3:30 CHEMICAL VAPOR DEPOSITION (CVD) BASED SYNTHESIS OF TIS, MICROSTRUCTURES USING TEMPLATE METHOD FOR SECONDARY LITHIUM BATTERIES, Guangli Che. Ellen R. Fisher, Kshama Jirage, Charles R. Martin, Colorado State University, Fort Collins, CO.
- 3:55 APPLICATION OF DIAMOND-LIKE CARBON THIN FILMS FOR CORROSION PROTECTION OF ALUMINUM SURFACES, Guangyuan Li, Greg M. Swain, Utah State University, Logan, UT.
- 4:20 FABRICA TION OF NANOTUBULAR MEMBRANES AND THEIR APPLICATION AS MOLECULAR FILTER, Kshams B. Jirage, Charles R. Martin, Colorado State University, Fort Collins, CO.

# SYMPOSIUM ON ENVIRONMENTAL CHEMISTRY

Organized by Maria W. Tikkanen Financial Support provided by Finnigan MAT

#### Monday, August 4, 1997

#### Morning Session: Maria W. Tikkanen, Presiding

- 8:30 Opening Remarks
- 8:35 INVITED SPEAKER IN ENVIRONMENTAL CHEMISTRY THE ACCURATE DETERMINATION OF SPECIES BY SPECIATED ISOTOPE DILUTION MASS SPECTROMETRY: EXEMPLIFIED BY THE EVALUATION OF CR (VI) IN SOIL, H.M. "Skip" Kingston. Dengwei Huo, Yusheng Lu, Duquesne University, Department of Chemistry and Biochemistry and the Environmental Science Program, Pittsburgh, PA 15282.

9:35 **INVESTIGATION OF URANIUM CONTAMINATION IN A GREA T LAKES HARBOR**, <u>Michael E.</u> <u>Ketterer</u>. Department of Chemistry, John Carroll University, University Heights, OH 44118; Ricky L. Layman, Gerald Matisoff, Chris Bonniwell, and Peter McCall, Department of Geological Sciences, Case Western University, Cleveland, OH 44106.

- 9:55 DEVELOPMENT OF AN IMPROVED METHOD FOR THE DETERMINATION OF ARSENIC AT LOW LEVELS IN BIOLOGICAL MA TRICES. <u>Ruth Hund</u>, American Water Works Association Research Foundation, 6666 W. Quincy Avenue, Denver, CO 80235, X. Chris Le, 13-103 Clinical Sciences Building, University of Alberta, Edmonton, AB T6G 2G3.
- 10:15 Break
- 10:35 LANL CMR ORGANIC ANALYSIS CAPABILITIES FOR ENVIRONMENTAL APPLICATIONS. Gerald B. Ansell. Michael E. Cournoyer, Kirk W. Hollis, Anthony Lombardo, and Peter C. Stark, MS G740, LANL, Los Alamos, NM 87545-0000."
- 10:55 MTBE IN GROUNDWATER AND SURFACE WATERS IN CALIFORNIA. Maria W. Tikkanen, Association of California Water Agencies, 910 K Street, Sacramento, CA 95814; R.G. Sykes, East Bay Municipal Water District, 375 Eleventh St., Oakland, CA 94607-4240.
- 11:15 VOLATILE METALS RECOVERY USING A TEMPERATURE CONTROLLED OPEN VESSEL MICROWAVE SYSTEM. James C. Price. CEM Corporation, P.O. Box 200, Matthews, NC 28106-0200.
- 11:35 ARSENIC SPECIATION IN ENVIRONMENTAL SAMPLES USING A VG PLASMAQUAD ICP-MS FOR ELEMENT-SPECIFIC DETECTION OF ION-PAIRING LC AND MICRO-LC SEPARATIONS. Mary Kate Donais, VG Elemental, 27 Forge Parkway, Franklin, MA 02038, Stephen E. Long National Institute of Standards and Technology, Gaithersburg, MD 20899.

#### Afternoon Session: Maria W. Tikkanen, Presiding

- 1:30 CONTAMINATED SEDIMENT REMEDIATION BY 'IN-SITU SAND CAPPING' IN HAMILTON HARBOUR, LAKE ONTARIO, CANADA. <u>Fernando Rosa</u>, National Water Research Institute, 867 Lakeshore Rd., Burlington, Ontario, Canada L7R 4A6.
- 1:55 THE USE OF MEDIA WITH HIGH DIELECTRIC CONSTANT FOR HAZARDOUS METAL ION SEPARATION. John D. Lamb and <u>Alexander Y. Nazarenko</u>, Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602-5700.
- 2:15 CHEMICAL IMAGING FOR ENVIRONMENTAL ANALYSIS. Israel Schechter. Department of Chemistry, Technion - Israel Institute of Technology, Haifa 32 000, Israel.
- 2:35 HIGH THROUGHPUT MICROWAVE SAMPLE PREPARATION OF SULFIDE ORE SAMPLES FOR ANALYSIS BY ICAP. Sara Littau. Doug Ferguson, CEM Corporation, P.O. Box 200, Matthews, NC 28106.
   2:55 Break
- 3:15 SPECTROSCOPIC DETERMINATION OF THE MOLECULAR COMPOSITION AND DIAGNOSTICS OF THE PULSED CORONA DISCHARGE. Sandra Poteat Shofran, and Charles B. Boss, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204; Phil A. Lawless, Research Triangle Institute, Research Triangle Park, NC 27709; G.H. Ramsey, U.S. Environmental Protection Agency, Research Triangle Park, N.C. 27709.
- 3:35 NEW CHELATING POLYMERS FOR SORPTION OF HEAVY METALS IONS FROM AQUEOUS SOLUTION. Richard A. Bartsch, <u>Galina G. Talanova</u>, and Longgui Zhong, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX 79409.
- 3:55 FORMATION OF PARTICLES LESS THAN ONE MICRON IN DIAMETER BY SUPERCRITICAL CARBON DIOXIDE-ASSISTED NEBULIZA TION. <u>CM. Karbiwnyk</u>. U. Karst, C.R. Stoldt, WA. Andersen, J.D. Schaefer, C. Xu, B.A. Watkins, and R.E. Sievers, CIRES, University of Colorado, CB 216, Boulder, CO 80309-0216.
- 4:15 To be announced

#### Tuesday, August 5,1997

#### Morning Session: Edward T. Furlong, Presiding

- 8:30 Opening Remarks
- 8:35 **INVITED SPEAKER IN ENVIRONMENTAL MASS SPECTROMETRY** Sponsored by Finnigan MAT. To be Announced
- 9:35 DESCRIBING NON-CONSTANT VARIANCE-A MODEL FOR ESTIMATING SAMPLING AND ANALYSIS PRECISION WITH APPLICATION TO ENVIRONMENTAL MEASUREMENTS. Jeffrey W. Pritt, U.S. Geological Survey, 5293 Ward Road, Arvada, Colorado 80002.
- 9:55 DETERMINATION OF LIMIT OF QUANTIFICATION FOR HEXACHLOROBENZENE IN SELECTED PRODUCTS AND SAMPLES. Chung H. Chiu, Mylaine Tardif, Viera Balgava and Gary Poole, Environment Canada, 3439 River Road, Environmental Technology Centre, Ottawa, Ontario, Canada K1A 0H3.
   10:15 Break

10:35 OCCURRENCEL MNDDEFISTRABIETEOSE OF MAGINATIONES OF A SUMMER OF A SUME OF A SU

10:55 DETERMINA TION OF PESTICIDES IN WATER BY STYRENE DIVINYL BENZENE SOLID-PHASE EXTRACTION AND HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY. Stephen L. Werner. Mark R. Burkhardt, and Bruce D. Anderson, U.S. Geological Survey, National Water Quality Laboratory, 5293 Ward Road, MS 407, Arvada, CO 80002.

11:15 To be announced

# 20<sup>™</sup> INTERNATIONAL EPR SYMPOSIUM

Organized by Sandra S. Eaton and Gareth R. Eaton Update information will be posted as it becomes available at http://www.du.edu/~seaton/eprsym.html Financial Support provided by: SPONSOR: Bruker Instruments, Inc., EPR Division CONTRIBUTORS include: Research Specialties Scientific Software Services Wilmad Glass

## Sunday, August 3,1997 - Open House at the University of Denver

5:45 pm Meet in hotel lobby for bus transportation.

- Bruker will present a brief overview of highlights of their exhibit.
- A buffet supper will be provided, compliments of Bruker.
- There will be demonstrations and exhibits of our spectrometers.

#### Monday, August 4,1997

#### Session I, W. Trommer presiding

- 8:30 Opening Remarks and Welcome, Gareth R. Eaton
- 8:35 ENDOR OF METALLOENZYME REACTIVE INTERMEDIATES, J.-P. Willems, H. I. Lee, P. Doan, B. Sturgeon, D. Burdi, J. Stubbe, and <u>B. M. Hoffman.</u> Northwestern University and MIT.
- 9:15 **POSITIONING OF PHOSPHOLIPASE A2 AT THE MEMBRANE SURFACE USING BARRIER-IMPEDED RELAXANT DIFFUSION EPR,** Y. Lin, R. Nielsen, M. H. Gelb, and <u>B. H. Robinson</u>. University of Washington.
- 9:45 **PULSE EPR AND ENDOR STUDY OF CO(II) PORPHYRIN COMPLEXES,** <u>S. E. Van Doorslaer</u> and A. Schweiger, ETH Zentrum, Switzerland.
- 10:05 Break
- 10:35 ENDOR AND HYSCORE CHARACTERIZATION OF FLAVOPROTEIN SEMIQUINONES IN RELATION TO PROTEIN FUNCTION, J. I. Martinez, A. Lostao, J. Sancho, R. Cammack, C. Gomez-Moreno, P. J. Alonso, and <u>M. Medina</u>. Universidad de Zaragoza, Spain.

# 11.00 ELECTRON MAGNETIC RESONANCE STUDIES OF PROTEIN-SOLVENT AND PROTEIN-

CHAPERONIN INTERACTIONS OF SPIN-LABELED MUTANTS OF HCA II, M. Lindgren. M. Persson, P. Hammarstrom, M. Svensson, U. Carlsson, B.-H. Jonsson, G. R. Eaton, and S. S. Eaton, Linkoping University, Sweden, Umea University, Sweden, and University of Denver.

11:20 CROSS PEAK INTENSITIES IN DEUTERIUM TWO-DIMENSIONAL FOUR PULSE SPIN ECHO MODULATION SPECTRA, A. Poppl and R. M. Bottcher, Universitat Leipzig, Germany.

11:40 ESR CHARACTERIZATION OF THE FRAMEWORK LOCATION OF COBALT ION IN COAPO-41 AND COAPSO-41 MOLECULAR SIEVES, A. M. Prakash, M. Hartmann, and L. Kevan. University of Houston and Universitat Stuttgart, Germany.

#### Session II, M. K. Bowman, presiding

- 1:30 *HIGH RESOLUTION EPR IMAGING USING NARROW LINE SPIN PROBES*, <u>H. J. Halpern.</u> G. V. R. Chandramouli, E. D. Barth, and B. Sturgeon, University of Chicago.
- 2 00 **PULSED RADIOFREQUENCY FT EPR SPECTROMETER/IMAGER FOR IN VIVO APPLICATIONS,** M. Afeworki, N. Devasahayam, J. Cook, R. Murugesan, S. Subramanian, R. Tschudin, J. B. Mitchell, and <u>M. C. Krishna</u>. NTH, Bethesda.

	, 5 5
2:30	DETERMINATION AND CHARACTERIZATION OF NITRIC OXIDE GENERATION IN MICE BY IN-
	VIVO L-BAND EPR SPECTROSCOPY, H. Fujii, J. Koscielniak, and L. J. Berliner. Ohio State University.
2:50	Break
<b>3</b> ;20	LIPID-MRI CONTRAST AGENT INTERACTIONS: A SPIN LABELING AND MULTIFREQUENCY EPR
	STUDY, T. I. Smirnova, A. I. Smirnov, R. L. Belford, and R. B. Clarkson, University of Illinois.
3:45	MOLECULAR MOTION AND CHEMISTRY IN ZEOLITE CAGES, D. C. Doetschman. J. D. Fox, G. D.
	Thomas, and D. W. Dwyer, SUNY-Binghamton and SUNY-Brockport.
4:10	IMIDAZOLINE NITROXIDES AS PROBES FOR LOCAL CHEMICAL ENVIRONMENT: EPR
	DETECTION OF PROTONS, THIOLS, AND NITRIC OXIDE, V. V. Khramtsov. Institute of Chemical
	Kinetics & Combustion, Russia.
4.35	DETECTION OF PROTEIN-DERIVED RADICALS FROM THE REACTION OF HORSERADISH
	PEROXIDASE AND LIGNIN PEROXIDASE WITH HYDROGEN PEROXIDE: AN EPR SPIN-TRAPPING
	STUDY, Y. C. Fann. S. D. Aust, and R. P. Mason, National Institutes of Environmental Health Science and Utah
	State University.
5.00	Conference Mixer and Instrument Exhibit

5:00 Conference Mixer and Instrument Exhibit

#### Tuesday, August 5,1997

- Session III, L. Berliner presiding
- 8:30 SUPEROXIDE FORMATION FROM ENDOTHELIAL NITRIC OXIDE SYNTHASE: AN ESR SPIN-TRAPPING INVESTIGATION IN A LOOP-GAP RESONATOR, J. Vasquez-Vivar, P. Martasek, N. Hogg, K. A. Pritchard, Jr., and <u>B. Kalyanaraman</u>. Medical College of Wisconsin and University of Texas Health Science Center.
- 9:00 **EPR STUDIES OF NITROSYL SPECIES IN INFLAMMATION** J. K. Shergill, A. Inalsingh, M. N. Hughes, A. Bune, T. E. Cook, A. H. V. Schapira, and <u>R. Cammack</u>. King's College London, U.K., St. Mary's Hospital Medical School, U. K., and Free Hospital School of Medicine, U.K.
- 9:25 OXIDATIVE DAMAGE OF NEUROBLASTOMA CELLS BY 6-FLUORDOPAMINE AS SOURCE OF OH-RADICALS, H.-M. Schlude, H. Kohle, G. Seitz, G. Bruchelt, V. A. Roginsky, and <u>H. B. Stegmann</u>, Universitat Tuebingen, Germany, and Russian Academy of Sciences.
- 9:50 Break Please take time to see the exhibits
- 10.35 LIGAND SPECIFIC OPENING OF A GATED PORIN CHANNEL, MEASURED BY ESR SPECTROSCOPY, X. Jiang, M. A. Payne, Z. Cao, S. B. Foster, J. B. Feix, S. M. C. Newton, and <u>P. E. Klebba</u>. University' of Oklahoma.
- 11:10 BIOREDUCTION OF TEMPONE AND SPIN-LABELED GENTAMICIN BY P. AERUGINOSA CELLS: EVALUATION OF THE RATE CONTROLLING STEP AND EFFECT OF ULTRASOUND, <u>N. Rapoport</u> and A. Smirnov, University of Utah and University of Illinois.
- 11:30 LIPID-PROTEIN INTERACTION IN R-3-HYDROXYBUTYRATE DEHYDROGENASE AS STUDIED BY ESR SPECTROSCOPY, D. Chelius, J. Moeller, A. R. Marks, J. O. McIntyre, S. Fleischer, J. G. Wise, and <u>W. E.</u> Trommer, University of Kaiserslautern, Germany, Mount Sinai School of Medicine, and Vanderbilt University.

Session IV, L. Belford presiding

- 1:30 TIME-RESOLVED EPR STUDIES OF HYDROGEN ABSTRACTION FROM SUGARS INCLUDING CYCLODEXTRINS, <u>M. G. Bakker</u> and M. N. Lehmann, University of Alabama.
- 2:00 MULTI-PHOTON CHEMICAL REACTIONS, CHIRALITY, AND VIBRONIC MOTIONS STUDIED BY ESR, S. Shih. Yuan-Tze Institute of Technology, Taiwan.
- 2:25 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

(Posters are listed alphabetically by presenting author)

A **TWO- AND THREE-DIMENSIONAL SPATIAL IMAGING USING PULSED RADIOFREQUENCY FT EPR**, <u>M. Afeworki</u>. M. C. Krishna, N. Devasahayam, S. Subramaman, J. B. Mitchell, and <u>J. A. Cook</u>, National Institutes of Health, Bethesda.

B ACTIVE SITE ANALOGUES OF CYTOCHROME P450 - CHARACTERIZATION OF THE LIGAND SPHERE BY PULSE EPR AND ENDOR TECHNIQUES, <u>R. Bachmann.</u> A. Schweiger, H. Aissaoui, and W.-D. Woggon, ETH Zentrum, Switzerland and University of Basel, Switzerland.

A ADSORPTION OF SPIN-LABELED CTAB ON SILICA SURFACES: STRONG BINDING SITES AND SURFACTANT ORIENTATION BY BROADENING, M. G. Bakker. G. L. Turner, and K. Zhang, University of Alabama.

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- B ILLINOIS EPR RESEARCH CENTER A HIGH FIELD AND MULTIFREQUENCY EPR USER FACILITY, R. L. Belford, R. B. Clarkson, P. G. Debrunner, M. J. Nilges, and A. I. Smirnov, University of Illinois.
   A AN INVESTIGATION OF ESEEM LINESHAPE AND ZEEMAN FIELD-DEPENDENCE FOR THE TWO PRINCIPAL TYPES OF NITROGEN ATOMS, C. Bender. Albert Einstein College of Medicine.
   B AN IMPROVED PROTOCOL FOR THE EXPERIMENTAL MEASURE OF THE LINEAR ELECTRIC
- FIELD EFFECT, C. Bender, Albert Einstein College of Medicine.
- A **PARAMAGNETIC CENTERS IN BOROPHOSPHOSILICATE AND PHOSPHOSILICATE GLASS THIN FILMS, C. A. Billman, M. Lillis, P. M. Lenahan, R. Fuller, H. Evans, and R. Paulsen, Pennsylvania State** University, Harris Semiconductor, and Motorolla Corporation.
- B HYPERFINE TENSORS FOR 1=1/2 NUCLEI BY CONTOUR LINESHAPE ANALYSIS. APPLICATION TO INORGANIC COMPLEXES AND PROTEIN ACTIVE SITES, M. K. Bowman and S. A. Dikanov, Pacific Northwest National Laboratory and Institute of Chemical Kinetics and Combustion, Russia.
- A **COPPER ACCUMULATION IN TISSUES AFTER ACUTE ETHANOL TREATMENT,** <u>W. Chamulitrat</u> and J. J. Spitzer, Louisiana State University Medical Center.
- B INTERACTION OF TOCOPHEROL AND FREE FATTY ACIDS IN MODEL PHOSPHOLIPID
   MEMBRANE: ANTIOXIDANT ACTIVITY OF VITAMINE, D. F. Church. T. R. Dugas, J. D. Blazier, and G. M. Pineda, Radical Technologies and Louisiana State University.
- A *LARGE MAGNITUDE HIGH SPIN TERMS: FACT OR FICTION?* <u>R. F. C. Claridge</u> and W. C. Tennant, University of Canterbury, New Zealand.
- B **DNP-ENHANCED MRI WITH CARBON CHARS,** <u>R. B. Clarkson.</u> B. M. Odintsov, P. J. Ceroke, and J. H. Ardenkjaer-Larsen, University of Illinois and Nycomed Innovation AB, Sweden.
- MAGNETIC FIELD DEPENDENCE OF EPR LINEWIDTHS IN AQUEOUS SOLUTIONS OF GD(III)
   (S=7/2) AND MN(II) (S=S/2) CHELATES, <u>R. B. Clarkson</u>. A. I. Smirnov, T. I. Smirnova, R. I. Konda, H. Kang, and R. L. Belford, University of Illinois.
- B *A TWO-DIMENSIONAL COMBINATION PEAK (2D-CP) EXPERIMENT,* <u>S. E. Van Doorslaer</u> and A. Schweiger, ETH Zurich, Switzerland.
- AMAGNETIC INTERACTIONS IN (COPPER-DIPEPTIDES)SALTS:CU".GLY-TRP ANDC^.TRP-GLY,A. J. da Costa Fillo, R. Calvo, and O. R. Nascimento, Instituto de Fisica de Sao Carlos, Brazil.
- B PHOSPHAFULVENE RADICAL ANIONS: ELECTROCHEMICAL GENERATION, EPR STUDY AND AB INITIO INVESTIGATIONS, M. Geoffroy. A. A. Badri, and M. Chentit, University of Geneva, Switzerland.
- A **IDENTIFICATION OF THE 4-GL UTAMYL RADICAL AS AN INTERMEDIATE IN THE CARBON SKELETON REARRANGEMENT CATALYZED BY COENZYME B**<sub>n</sub>-**DEPENDENT GLUTAMATE MUTASE**, <u>G. J. Gerfen</u>. H. Bothe, D. J. Darley, S. P. J. Albracht, B. T. Golding, and W. Buckel, MIT, Philipps-Universitat, Germany, University of Newcastle upon Tyne, U. K., and BioCentrum Amsterdam, The Netherlands.
- B <sup>51</sup>VESE-ENDOR INVESTIGATION OF VANADYL MODEL COMPLEXES, <u>C. Grant.</u> J. Ball, R. D. Britt, B. Hamstra, and V. Pecoraro, University of California Davis and University of Michigan.
- A EPR INVESTIGATION OF AZIDE AS AN INHIBITOR OF OXYGEN EVOLUTION IN PHOTOSYSTEM II, R. A. Kimel, S. Stinson, and <u>A. Haddy</u>, UNC-Greensboro.
- B MODELS OF THE INTRACELLULAR AND EXTRACELLULAR TISSUE WATER: IMPLICATIONS FOR EPR MICROVISCOSITY MEASUREMENTS, H. J. Halpern and E. D. Barth, University of Chicago.
- A EPR AND X-RA Y CRYSTALLOGRAPHIC STUDIES OF DIMETHYLSULFOXIDE REDUCTASE FROM RHODOBACTER CAPSULATUS: IMPLICATIONS FOR CATALYSIS AND ELECTRON TRANSFER, I. Lane, P. S. Solomon, A. S. McAlpine, <u>G. R. Hanson.</u> S. Bailey, and A. McEwan, University of Queensland, Australia
- B THE DETERMINATION OF THE DISTANCES BETWEEN PARAMAGNETIC SPECIES IN PHOTOSYSTEM II STUDIED BY PULSED ELDOR AND "2+1" ESE METHODS, <u>H. Hara</u>. K. Shigemori, A. V. Astashkin, and A. Kawamori, Kwansei Gakuin University, Japan.
- A PULSED EPR STUDIES OF THE (CH.), CCOOH RADICAL FORMED BY 'IRRADIATION OF a-NH, ISOBUTYRIC ACID AND DI-METHYL-MALONIC ACID, J. R. Harbridge. S. S. Eaton, and G. R. Eaton, University of Denver.
- B **EPR STUDIES OF LEAD MAGNESIUM NIOBATE PIEZOELECTRICS,** <u>J. Huang</u>. M. Benjamin, and J. J. Fitzgerald, South Dakota State University.
- A **THE INFLUENCE OF FE<sup>-</sup> ON TJ OF THE PRIMARY REACTANTS (D , I , Q , Q ) IN REACTION CENTERS FROM PHOTOSYNTHETIC BACTERIA**, R. Calvo, <u>R. A. Isaacson</u>. E. C. Abresch, and G. Feher, University of California - San Diego.
- B **POLYNUCLEAR COPPER COMPLEXES INVESTIGATED BY HIGH-FREQUENCY EPR**, <u>H. KaB</u>. E. Goovaerts, A. Bouwen, D. Schoemaker, and R. E. P. Winpenny, University of Antwerp, Belgium, and University of Edinburgh, U. K.

	et al.: 39th RMCAC Preliminary Program and Registration Information
A	QUANTITATIVE DETERMINATION OF THIOLS USING NEW DISULFIDE IMIDAZOLIDINE
	BIRADICAL, V. Khramtsov, V. Yelinova, Yu. Gluzachev, and V. Reznikov, Institute of Chemical Kinetics &
	Combustion, Russia.
В	PHOTOINDUCED ELECTRON TRANSFER BETWEEN CAROTENOIDS AND SOL VENT MOLECULES,
	T. A. Konovalova, V. V. Konovalov, and L. D. Kispert, University of Alabama.
A	ESR OF MO(V) DISPERSED IN POLYMER MATRICES, K. Kruczala. K. Dyrek, and S. Schlick, University
	of Detroit Mercy.
В	2D SPATIAL-SPECTRAL ESR IMAGING BASED ON MO(V), K. Kruczala. Z. Gao, and S. Schlick,
	University of Detroit Mercy.
А	DPPH AS A STANDARD IN HIGH FIELD EPR SPECTROSCOPY, J. Krzvstek. A. Sienkiewicz, L. Pardi, M.
	Rohrer, and L. C. Brunei, National High Magnetic Field Laboratory and Polish Academy of Sciences, Poland.
В	EPR SPECTRA FROM "EPR-SILENT" SPECIES: HIGH FIELD EPR SPECTROSCOPY OF

*MANGANESE(III) PORPHYRINS,* D. P. Goldberg, J. Telser, <u>J. Krzystek</u>. L. C. Brunei, A. G. M. Barrett, and B. M. Hoffman, Northwestern University, National High Magnetic Field Laboratory, and Imperial College London, U.K.

Tuesday evening - EPR Symposium dinner. All attendees are invited, see information on http://www.du.edu/~seaton/eprsym.html

#### Wednesday, August 6,1997

Session VI, L. Kevan presiding

- 8:30 HIGH-FIELD EPR IN THE INVESTIGATION OF LOW-DIMENSIONAL MOLECULAR MAGNETIC MATERIALS, L. Pardi, L.-C. Brunei, A. Caneschi, and D. Gatteschi, National High Magnetic Field Laboratory and University of Florence, Italy.
- 8:55 MULTIFREQUENCY HIGH FIELD EPR SPECTROSCOPY OF CANTED ANTIFERROMAGNETS, G. Fanucci, J. Krzvstek. D. R. Talham, and L. C. Brunei, Florida State University and University of Florida.
   9.20 TIME EVOLUTION OF THE ESR SPECTRUM IN A METAL-INSULATOR TRANSITION SUPPRESSION, O. R. Nascimento, E. C. Pereira, A. Pawlicka, L. O. S. Bulhoes, and L. Walmslev. Universidade de Sao Paulo,
- Universidade Federal de S. Carlos, and Universidade Estadual Paulisa, Brazil.
   9:40 FABRICA TION, SPATIAL, AND SPIN CHAIN STRUCTURE OF LANGMUIR-BLODGETT FILMS OF COPPER TETRA-4-TERT-BUTYL PHTHALOCYANINE, Y. Shimoyama. T. Komatsu, and T. Takamura, Hokkaido University of Education, Japan.
- 10:00 Break

10:30 A PHYSICALLY BASED PREDICTIVE MODEL FOR E' GENERATION IN AMORPHOUS SIO, FILMS ON SILICON, P. M. Lenahan, B. D. Wallace, and J. F. Conley, Jr., Pennsylvania State University and Dynamics Research Corporation.

- 10:55 A NEW INTERPRETATION OF CR\* SPIN-LATTICE RELAXATION DATA IN CU^R^N^ SPINEL: ROLE OF EXCHANGE INTERACTION, S. K. Misra, Concordia University, Canada.
- 11:15 TIME DOMAIN EPR, 2D-ESEEM AND CW-ENDOR MEASUREMENTS OF NI(I) AND NI(III) TETRACYANIDES IN NACL AND KCL HOST LATTICES, N. V. Vugman. J. A. Coelho Neto, and N. M. Pinhal, Universidade Federal do Rio de Janeiro, Brazil.
   11.35 COMPUTER SIMULATION OF MAGNETIC RESONANCE SPECTRA EMPLOYING HOMOTROPY, K. E.
- <u>Gates</u>, G. R. Hanson, and K. Burrage, University of Queensland, Australia.

#### Session VII, P. M. Lenahan presiding

- 1 30 THE PERFORMANCE OF A SECOND GENERATION FT-EPR SPECTROMER, P. Hofer, Bruker Instruments, Germany.
- 2.00 ELECTRICALLY DETECTED MAGNETIC RESONANCE IN SI/SI» 7 GE ^ HETEROSTRUCTURES, <u>C. F.</u> <u>O. Graeff.</u> M. Holzmann, M. S. Brandt, M. Stutzmann, and F. Schaffler, University of Sao Paulo, Brazil, Technical University Munchen, Germany, and Daimler-Benz AG, Germany.
- 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
  - (Posters are listed alphabetically by presenting author)
- C EPR INVESTIGATIONS OF NITROUS OXIDE DECOMPOSITION ON RUTHENIUM AND COPPER ION-EXCHANGED ZEOLITES, P. J. Carl and <u>S. C. Larsen</u>, University of Iowa.

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- D NITRIC OXIDE SYNTHASE ACTIVITY IN THE SALIVARY GLANDS OF THE TICK DERMACENTOR VARIABILIS, S. T. Bhattacharya, <u>R. V. Lloyd</u>, W. Lamoreaux, N. Bayakly, M. Fitzgerald, and L. B. Coons, University of Memphis.
- C NANOMOLAR ALIQUOTS OF VOLA TILE SPIN PROBES IN EPR/UV TISSUE CELLS, K. Lo. S. L. Ticer. and W. Z. Plachy, San Francisco State University
- D A NOVEL LOADING-TOLERANT LARGE HOMOGENEOUS VOLUME L-BAND RESONATOR DESIGN FOR IN-VIVO EPR SPECTROSCOPY AND IMAGING, J. A. B. Lohman. A. M. Allan, A. W. Miller, A. J. Illsley, and R. Ladbury, Buker Spectrospin Limited, U. K.
- C AN IN SITU RADIOLYSIS ESR STUDY OF SPIN TRAPPING BY NITRONES: THE EFFECT OF INTRAMOLECULAR INTERACTIONS ON SPIN ADDUCT STABILITY IN AQUEOUS SOLUTION, <u>K. P.</u> <u>Madden</u> and H. Taniguchi, University of Notre Dame.
- D PLATFORM-INDEPENDENT EPR DATA ACQUISITION: IMPLEMENTATION IN WINDOWS, <u>R. Morse</u>. Illinois State University.
- C EFFECT OF NITROXIDES ON CELL GROWTH AND DEVELOPMENT, <u>R. Morse. L. Pham. W. Brix</u>. J. <u>Cianfrogna</u>. and <u>G. Martino</u>. Illinois State University.
- D **EXPERIMENTAL CONDITIONS FOR USE OF NITROXIDE IN CELL STUDIES,** <u>R. Morse.</u> A. I. Smirnov, D. T. Donovan, and K. A. Dickerson, Illinois State University and University of Illinois.
- C SOLVENT EFFECT IN AQUEOUS HARDWOOD CHARS SUSPENSIONS, <u>B. M. Odintsov</u>. P. J. Ceroke, R. L. Belford, A. B. Odintsov, and R. B. Clarkson, University of Illinois.
- D MOLECULAR MOTION AND DNP ENHANCEMENT IN AQUEOUS CHARS SUSPENSIONS. <u>B. M.</u> <u>Odintsov</u>, P. J. Ceroke, R. L. Belford, A. B. Odintsov, and R. B. Clarkson, University of Illinois.
- C DISTANCE LIMITATIONS AND NITROXIDE PROBE PAIR INTERACTIONS IN HELICAL DNA AN ESR STUDY, <u>T. M. Okonogi</u>. A. W. Reese, S. C. Alley, E. A. Harwood, P. B. Hopkins, B. H. Robinson, University of Washington.
- D DESIGN OF A HIGH PERFORMANCE SURFACE-COIL-TYPE RESONATOR FOR THE STRIATUM OF RAT FOR THE BRAIN FUNCTION STUDY, M. Ono. T. Yamura, H. Hirata, M. Hiramatsu, Yamagata University, Japan.
- C EPR AND ENDOR OF FREE RADICAL TAGGANTS, <u>M. D. Pace</u> and J. Joseph, Medical College of Wisconsin.
- D GENERAL THEORY OF THE RELAXA TION PROCESSES FOR MULTILEVEL SPIN SYSTEMS IN DILUTE PARAMAGNETIC SOLIDS AT HIGH TEMPERATURE, <u>F. F. Popescu.</u> University of Bucharest, Romania.
- C OFF-AXIS EXTRA LINES IN POWDER PATTERN EPR OF CHROMIUM IONS IN YTTRIUM ORTHOALUMINATE LASER CRYSTALS, <u>R. R. Rakhimov</u>, A. L. Wilkerson, G. B. Loutts, and H. R. Reis, Norfolk State University.
- D **TWO NEW HOLE-BURNING EXPERIMENTS WITH HIGH TURNING ANGLES,** J. J. Shane and A. Schweiger, ETH Zentrum, Switzerland.
- C **PULSE EPRAT Q-BAND FREQUENCIES**, J. J. Shane. R. Rakhmatouline, J. Forrer, and A. Schweiger, ETH Zentrum, Switzerland.
- D A NEW SPIN DENSITY EQUATION FOR NON-PLANAR CATION RADICALS OF ETHYLENE AND ITS ALKYL DERIVATIVES, S. Shih. Yuan-Tze Institute of Technology, Taiwan.
- C **RAPID SCAN DIELECTRIC RESONATOR-BASED FLOW AND STOPPED-FLOW EPR,** <u>A. Sienkiewicz</u>. A. M. da Costa Ferreira, H. Taylor, R. E. Hansen, and C. P. Scholes, Polish Academy of Sciences, Poland, SUNY-Albany, and Universidade de Sao Paulo, Brazil.
- D COMPARATIVE SPIN-LABEL SPECTRA ATX-BAND (9.5 GHZ) AND W-BAND (95 GHZ), <u>A. I. Smirnov.</u> R. L. Belford, R. B. Clarkson, T. I. Smirnova, and M. J. Nilges, University of Illinois.
- C ORIENTED SELF-ASSOCIATION OF COPPER(II) TETRAPHENYLPORPHINE IN LIPID BILAYER MEMBRANES: AN EPR SPIN LABELING STUDY, W. K. Subczvnski. M. Pasenkiewicz-Gierula, and W. E. Antholine, Medical College of Wisconsin and Jagiellonian University, Poland.
- D **FERRITIN TEMPERATURE DEPENDENCE STUDY,** <u>E. Wajnberg.</u> <u>D. M. S. Esauivel</u>. and L. J. El-Jaick, Centra Brasileiro de Pesquisas Fisicas, Brazil, and CECIERJ, Brazil.
- C MEASUREMENT OF INTERSPIN DISTANCE BY TIME-DOMAIN EPR OF SPIN-LABELED METMYOGLOBIN MUTANTS, <u>Y. Zhou.</u> B. Bowler, S. S. Eaton, and G. R. Eaton, University of Denver.

Wednesday evening - Chinese dinner, see poster area for details.

#### Thursday, August 7,1997

Session IX, L.-C. Brunel, presiding

- 8:30 SOLID-LIQUID SCALAR INTERACTIONS IN AQUEOUS CHARS SUSPENSIONS BY PULSED DNPAT LOW MAGNETIC FIELD, <u>B. M. Odintsov</u>. P. J. Ceroke, R. L. Belford, and R. B. Clarkson, University of Illinois.
- 9:00 *TIME-RESOLVED EPR IN HIGH MAGNETIC FIELDS*, <u>H. P. Moll</u>. J. van Tol, A. Witowski, C. Kutter, and P. Wyder, Grenoble High Magnetic Field Laboratory, France.
- 9:30 TODAYS PERFORMANCE STANDARDS OF A W-BAND EPR SPECTROMETER, G. C. Maresch. P. Hofer, and D. Schmalbein, Bruker Instruments, Germany.

- 10:20 **PROPOSAL FOR A NEW MULTIPLE RESONANCE TECHNIQUE: THE SPECTROSCOPIC BRIDGE, F** <u>F. Popescu</u>. University of Bucharest, Romania.
- 10:50 DIRECTLY MEASURING LONGITUDINAL ELECTRON SPIN RELAXATION: PRINCIPLES AND
- APPLICATIONS, <u>V. A. Atsarkin.</u> V. V. Demidov, and G. A. Vasneva, Russian Academy of Sciences, Moscow.
   APPLICATION OF TWO DIMENSIONAL FOURIER TRANSFORM ESR TO MODEL MEMBRANES, R,
- H. Crepeau. P. P. Borbat, and J. H. Freed, Cornell University.
- 11:50 Closing Remarks Sandra S. Eaton
- Thursday lunch and afternoon: Bruker User's Group. Please register at the Bruker booth in the exhibit area and contact Dr. Arthur Heiss for information about location and program. Also visit http://www.bruker.com and browse the EPR section.

# SYMPOSIUM ON FTIR/NIR/RAMAN SPECTROSCOPY

Organized by Abdul R. Chughtai and Dwight Smith

Financial support provided by ASI Applied Systems, Millersville, MD.

#### Monday, August 4,1997

- Session I, Abdul R. Chughtai, presiding
- 8:35 EFFECT OF OXIDANTS AND SUBSEQUENT HYDRATION ON BLACK CARBONS AND CARBON BLACKS. Abdul R. Chughtai and Dwight M. Smith, Department of Chemistry and Biochemistry, University of Denver, Denver, CO 80208.
- 9:05 *FLEXING THE DIRECTION OF INSTRUMENTATION*, <u>W. G. Fatelev.</u> R. A. DeVerse, and R. M. Hammaker, Department of Chemistry, Kansas State University, Manhattan, KS 66506-3701.
- 9.30 DEVELOPMENT OF SILANE-MODIFIED GOLD COLLOID ARRAY SUBSTRATES FOR INVESTIGATING SURFACTANT ADSORPTION KINETICS WITH SERS, Lydia G. Olson and Joel M. Harris, Department of Chemistry, University of Utah, SLC, UT 84112.
- 10:00 Break
- 10:15 ANALYSIS OF THE OILS AND GREASE COMPONENT OF A WASTEWATER TREATMENT FACILITY INFLUENT AND EFFLUENT USING FTIR Philip A. Russell, L/E WWTP, Englewood, CO 80110.
- 10:40 CHEMICAL MAPPING USING TWO DIMENSIONAL HADAMARD TRANSFORM RAMAN SPECTROMETRY, <u>R. A. DeVerse</u>. T. A. Mangold, R. M. Hammaker, and W. G. Fateley, Department of Chemistry, Kansas State University, Manhattan KS. 66506-3701.
- 11:05 **VIBRATIONAL MICROSPECTROSCOPY OF INORGANIC SOLIDS AT HIGH EXTERNAL PRESSURES,** Stephanie D. Warner. Ian S. Butler and Ivor Wharf, Department of Chemistry, McGill University, 801 Sherbrooke St. West, Montreal Quebec, Canada H3A2K6.
- 11:30 INNOVATIVE SOLUTIONS FOR PHARMACEUTICAL ANALYSIS USING FT-RAMAN AND FTIR TECHNIQUES, Ben Garland and Bill Moher, Nicolet Instrument Corporation, 355 River Oaks Parkway, San Jose, California 95134.

<sup>10:00</sup> Break

# Rocky Mountaig Entering of Moster Bymposydim 9 [1997], Art. 1

Organized by Mary E. Cast

## (Posters are listed aphabetically by presenting author)

- MANGANESE III CHEMICAL OXYGEN DEMAND PROCEDURE, Wayne T. Bovles. Hach Company, P.O. Box 389, Loveland, CO 80539-0389.
- 2 INFRARED AND RAMAN SPECTRA OF TETRACALCIUM PHOSPHATE, Ajit Jillavenkatesa and <u>Robert A.</u> <u>Condrate</u>, Sr., New York State College of Ceramics, Alfred, NY 14802.
- 3 ANALYSIS OF PRECONCENTRATED ACTINIDES IN BRINE SOLUTIONS USING ICP-MS, Julie A. Eyre. Sandra L. Bonchin, La Verne A. Gallegos, Thomas M. Yoshida, Los Alamos National Laboratory, CST-9, MS G740, Los Alamos, NM 87545.
- 4 SOLID-STATE AMPEROMETRIC DETECTOR OF GAS-PHASE HYDROGEN PEROXIDE, <u>Scott D.</u> Holmstrom. James A. Cox, Department of Chemistry, Miami University, Oxford, OH 45056.
- 5 SPE CLEANUP AND HPLC/UVDETECTION OF DECOQUINA TE IN FEEDS, Jeffrey A. Hurlbut\*. Peter A. Perrone\*, Joseph M. Storey\*, J. David Bradley\*, and Calvin C. Walker\*, \*Chemistry Department, Metropolitan State College of Denver, P.O. Box 173362, Denver, CO 80217, \*Food and Drug Administration, Denver Federal Center, P.O. Box 25087, Denver, CO 80225.
- 6 HPLC/UV DETERMINATION AND SPE CLEANUP OF EPHEDRA ALKALOIDS IN DIETARY PRODUCTS, Jeffrey A. Hurlbut\*. Barbara S. Portz\*, Kent C. Faul\*, Jennifer C. Pensoneau\*, \*Chemistry Department, Metropolitan State College of Denver, P.O. Box 173362, Denver, CO 80217, \*Food and Drug Administration, Denver Federal Center, P.O. Box 25087, Denver, CO 80225.
- 7 ANALYSIS OF NITROAROMATIC AND NITRAMINE EXPLOSIVES IN SURFACE WATERS USING LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY (LC-MS), Stuart A. Oehrle. Waters Corporation, 34 Maple St., Milford, MA 01757.
- 8 ANALYSIS OF DEGRADATION PRODUCTS OF CHEMICAL WARFARE AGENTS IN ENVIRONMENTAL MATRICES BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY(HPLC-MS), Stuart A. Oehrle. Waters Corporation, 34 Maple St., Milford, MA 01757.
- 9 ANALYSIS OF BENZODIAZEPINES IN WHOLE BLOOD BY LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY (LC-MS), Stuart A. Oehrle. Waters Corporation, 34 Maple St., Milford, MA 01757.
- A NEW WASTE MINIMIZATION METHOD FOR THE DETERMINATION OF TOTAL NONHALOGENATED VOLATILE ORGANIC COMPOUNDS IN TRU WASTES, Walter F. Sandoval, Michael E. Cournoyer, Laura C. Ortega, Leah D. Bustos, MS G740, CST-12, Los Alamos National Laboratory, Los Alamos, NM 87545.
- U CARBONATE AND ORGANIC CARBON ASSOCIATED WITH COLLOIDS IN THE MISSISSIPPI RIVER AND MAJOR TRIBUTARIES, Colleen E. Rostad. John R. Garbarino, U.S. Geological Survey, MS 408, 5293 Ward Road, Arvada, CO 80002.
- 12FATE ANDTRANSPORT OFTOTALORGANIC HALIDE IN AWETLAND AREA,Barbara J.Stricos.Colleen E. Rostad, Larry B. Barber, U.S. Geological Survey, MS 408, 5293Ward Road, Arvada, CO80002.
- 13 A FIL TRA TION-BASED TECHNOLOGY FOR COPPER SEPARA TIONS IN ELECTROPLA TING RINSE WATERS, <u>Stephen M. Truiillo</u>, Michael E. Cournoyer, Reanna Aguino, MS G740, CST-12, Los Alamos National Laboratory, Los Alamos, NM 87545.
- 14 CONFIRMATION OF FLUOROQUINOLONES IN MILK AND CATFISH TISSUE BY ELECTROSPRAY LC/MS, Sherri B. Turnipseed. Jose E. Roybal, Allen P. Pfenning, Calvin C. Walker, FDA, Animal Drugs Research Center, Denver Federal Center, Bldg. 20, Denver, CO 80225-0087.
- 15 DEVELOPMENT OF SOLID-STATE ELECTROCATALYTIC SYSTEMS FOR APPLICATIONS TO AMPEROMETRIC SENSORS, <u>Anna Wolkiewicz</u>. Krzysztof Miecznikowski, James A. Cox, Chemistry Department, Miami University, Oxford, OH 45056.

# LUMINESCENCE SYMPOSIUM

Organized by: DeLyle Eastwood and Robert J. Hurtubise

## Monday, August 4,1997

#### Morning: Robert J. Hurtubise, Presiding

- 8:30 **Opening Remarks**
- 8:35 CHARACTERIZATION OF BENZO(A)PYRENE-DNA ADDUCTS BY SOLID-MATRLX LUMINESCENCE LIFETIMES, R.J. Hurtubise and Y. Chu, Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838.

- 8:55 **DETERMINATIONS 90% BMOXO (Prithmins by ADDI)** aff Sand Rogist Addorright Science, Ming Li and Robert J. Hurtubise, Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838.
- 9:15 SEPARATION OF PAH METABOLITES USING GAMMA-CYCLODEXTRIN MODIFIED MICELLAR ELECTROKINETIC CHROMATOGRAPHY WITH LASER-INDUCED FLUORESCENCE DETECTION, Christopher J. Smith. James Grainger, and Donald G. Patterson, Jr., Centers for Disease Control and Prevention, 4770 Buford Hwy., MS F-17, Atlanta, GA 30341.
- 9:35 **ENVIRONMENTAL MONITORING USING NEAR-INFRARED FLUOROPHORES**, Lawrence Evans III. Koen Van Aken, Lucjan Strekowski, and Gabor Patonay, Department of Chemistry, Georgia State University, University Plaza, Atianta, GA 30303.
- 9:55 TIME-RESOLVED LUMINESCENCE MONITORING OF INTERMEDIATES IN PHOTOINITIATED FREE-RADICAL KINETICS, Stephanie R. Shield and Joel M. Harris, Department of Chemistry, University of Utah, Salt Lake City, UT 84112.

10:15 Break

- 10:40 NON-PARAMETRICANALYSIS OF PYRENE PHOTOKINETICS BY DYNAMIC MULTIDIMENSIONAL FLUORESCENCE SPECTROSCOPY, Sharon L. Neal and Michele Villegas, Department of Chemistry, University of California, Riverside, CA 92521.
- 11:00 LUMINESCENCE STUDIES OF A NEW CLASS OF RE(1) POLYPYRIDINE COMPLEXES CONTAINING CIS-CARBONYL LIGANDS, Erick Schutte, Jeffrey B. Helms. Stephen Woessner, John Bowen, and B. Patrick Sullivan, Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838.
- 11.20 IMPROVED PERFORMANCE OF POLYMERIC ENCAPSULANTS AGAINST UV-INDUCED DISCOLORATION CHARACTERIZED BY SPECTROPHOTOMETRIC ANALYSES, F.J. Pern and S.H. Glide Center for Performance Engineering and Reliability, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401.

#### Afternoon Session: Jim Gord and DeLyle Eastwood, CO-chairs

- DeLyle Eastwood, presiding
- 2:00 **Opening remarks**
- 2:05 INTERACTIONS OF POLYMERS WITH LUMINESCENT METAL COMPLEXES AND ORGANIC DYES. DESIGN OF USEFUL ANALYTICAL SYSTEMS, J.N. Demas. Wenying Xu, and Kristi Kneas, Department of Chemistry, University of Virginia, Charlottesville, VA 22901; B.A DeGraff, Department of Chemistry, James Madison University, Harrisonburgy, VA 22807.
- 2:25 AUTOMATED TEST APPARATUS FOR QUENCHED-LUMINESCENCE SENSORS, <u>Alan E. Baron.</u> Sheldon Danielson, Tim M. Hance, and Thanachai Amnajanan, PhotoSense LLC, 1180 S. Flatiron Ct., Ste. B., Boulder, CO 80301.
- 2:45 THE USE OF LUMINESCENT SPECIES FOR AERODYNAMIC MEASUREMENTS, Patricia Coleman. Ford Motor Company, P.O. Box 2053, Mail Drop 3083/SRL, Dearborn, MI 48121-2053.
- 3:05 CONTINUING DEVELOPMENT OF LUMINESCENCE TECHNIQUES FOR CHARACTERIZING AVIATION FUEL, James R. Gord. Aero Propulsion and Power Directorate, Wright Laboratory, Wright-Patterson Air Force Base, OH 45433-7103; Keith D. Grinstead, Jr. and William L. Weaver, Innovative Scientific Solutions, Inc., 3845 Woodhurst Court, Beavercreek, OH 45430-1658.
- 3:25 Break
- 3:45 AERODYNAMIC PRESSURE AND TEMPERATURE MEASUREMENT THROUGH FLUORESCENCE LIFETIME IMAGING, Keith D. Grinstead. Jr., Larry P. Goss, and Darryl D. Trump, Innovative Scientific Solutions, Inc., 3845 Woodhurst Court, Beavercreek, OH 45430-1658; James R. Gord, Aero Propulsion and Power Directorate, Wright Laboratory, Wright-Patterson Air Force Base, OH 45433-7103.

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DEVELOPMENT OF SOL-GEL-DERIVED PRESSURE-SENSITIVE COATINGS FOR LIFETIME-BASED IMAGING, Jeffrey D. Jordan and Frank V. Bright, Department of Chemistry, Natural Sciences Complex, State University of New York at Buffalo, Buffalo, NY 14260-3000; Larry P. Goss, William L. Weaver, and Keith D.

Grinstead, Jr., Innovative Scientific Solutions, Inc., 3845 Woodhurst Court, Beavercreek, OH 45430-1658; James R. Gord, Aero Propulsion and Power Directorate, Wright Laboratory, Wright-Patterson Air Force Base, OH 45433-7103.

#### 4:25 USE OF FLUORESCENCE LIFETIMES OF INTRAMOLECULAR EXCIMER FORMERS FOR TEMPERATURE MEASUREMENT IN LIQUIDS, <u>Steven W. Buckner</u> and R Alan Forlines, Department of Chemistry and Geology, Columbus State University, Columbus, GA 31907 and James R Gord, Wright Laboratory Aero Propulstion and Power Directorate, Wright-Patterson Air Force Base, OH 45433.

# SYMPOSIUM ON MASS SPECTROMETRY

Organized by Joseph A. Zirrolli

Afternoon: Tuesday, August 5,1997

To be anounced

4:05

# SYMPOSIUM ON NMR SPECTROSCOPY

NMR Abstracts available at http://www.cchem.berkeley.edu/~jargrp/rmc.html Organized by L. Frydman, C. Grey, J. Hanna, J. Reimer, S. Sinton, R Wind and J. Yesinowski

## Monday, August 4,1997

#### Session I: New Techniques and Applications

Clare Grey, Presiding

- 8:25 Welcoming Remarks, James Yesinowski
- 8:30 HIGH RESOLUTION NMR SCATTERING, W. Zhang and <u>D. G. Cory</u>. Department of Nuclear Engineering, Massachusetts Institute of Technology, NW14-4111, 150 Albany St., Cambridge, MA 02139.
- 9:00 **SEDOR CAN COUNT SPINS,** <u>T. Gullion</u> and M. S. Conradi, Department of Chemistry, Department of Physics, Washington University, St. Louis, MO 63130.
- 9:30 COHERENT AVERAGING THEORY AND CHEMICAL SHIFT MEASUREMENTS: HOW GOOD ARE THE APPROXIMATIONS?, H. Cho, EMSL P7-55, Pacific Northwest National Laboratory, P. O. Box 999, Richland, Washington 99352.

10:00 Break

- 10:30 NMR STUDIES OF ADSORBATES ON COMMERCIAL FUEL CELL ELECTRODES IN AN AQUEOUS ENVIRONMENT, B.M. Rush, M. S. Yahnke, J.A. Reimer. E.J. Cairns, Energy and Environment Division, Lawrence Berkeley National Laboratory and Department of Chemical Engineering, University of California at Berkeley, Berkeley, CA 94720.
- 11:00 IN SITU SOLID STATE NMR STUDIES OF HETEROGENEOUS ENVIRONMENTAL PHOTOCATALYSIS, D.Raftery. S.-J. Hwang and C. Petucci, Department of Chemistry, Purdue University, West Lafayette IN 47907.
- 11:30 HYDROGEN BONDING AND EXCHANGE IN SUPERCRITICAL WATER AND ALCOHOLS, M.M. Hoffmann and M. S. Conradi, Washington University-1105, Departments of Physics and Chemistry, One Brookings Drive, St. Louis, Missouri 63130.

## Monday, August 4,1997

Session II, Poster Session A (Odd-numbered posters will be presented.)

Robert Wind, Presiding

( Posters listed in alphabetical order of presenting author.)

1:30-3:00

- 1. MULTIPLE INTERNUCLEAR COUPLINGS, ISOTROPIC TRANSFORMS, AND PURE DIPOLAR SPECTRA, D. J. Aurentz. J. M. Gibson, M. D. Karra, F. G. Vogt and K.T. Mueller, Department of Chemistry, The Pennsylvania State University, 152 Davey Laboratory, University Park, PA 16802-6300.
- 2. *MULTIPLE QUANTUM FILTERING AND SPIN EXCHANGE IN SOLID STATE NMR,* Yong Ba and J.A. Ripmeester, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, K1A OR9, Canada.
- 3. LIFE AT LOW GAMMA, HIGH SPIN AND LOW ABUNDANCE: SOLID STATE "'\*" TI AND """MO NMR, <u>T.J.Bastow</u>. Materials Science and Technology, CSIRO, Locked Bag 33, S.Clayton MDC, Clayton, Victoria 3169, Australia.

- 4. EXAMINATION OF THE DYNAMICS OF SOLVENT-SOLUTE INTERACTIONS BY MONITORING PARAMAGNETIC SPECIES-INDUCED 'H AND 'H RELAXATION BEHAVIOR, R.D. Bates. Jr.. Department of Chemistry, Georgetown University, Washington, DC 20057.
- 5. INVESTIGATION OF PARTIAL OXIDATION CATALYSTS BY SOLID-STATE NMR, J.M. Bemis. M.C. Douskey and E.J. Munson, University of Minnesota, 207 Pleasent St. S.E., Minneapolis, MN 55455.
- 6. THE USE OF LASER-POLARIZED XENON IN SURFACE NMR UNDER MAGIC ANGLE SPINNING CONDITIONS, E. Brunner. R. Seydoux, M. Haake and A. Pines, Materials Sciences Division, Lawrence Berkeley National Laboratory and the Departments of Chemistry and Chemical Engineering, University of California, Berkeley, CA, 94720.
- 7. LONG RANGE C-H DIPOLAR COUPLINGS IN LIQUID CRYSTALS MEASURED BY MULTI-DIMENSIONAL NMR EXPERIMENTS, <u>S. Caldarelli</u>. A. Lesage and L. Emsley, Institut de Recherches sur la Catalyse- CNRS, 69626 Villeurbanne, France; Ecole Normale Superieure de Lyon, 69364 Lyon, France.
- 8. STUDY OF THE SOLID-STRUCTURE AND THE MOLECULAR MOBILITY OF POLYPROPYLENE AND ETHYLENE-PROPYLENE BLOCK COPOLYMERS BY NMR, C. Jansen, P. Adriaensens, J. Gelan and R <u>Dommisse</u>. Ruca Groenenborgerlaan, 171, 2020 Antwerp, Belgium; (2) LUC, Universitaire Campus, Gebouw D, 3590 Diepenbeek, Belgium.
- 9. HIGH-RESOLUTION SOLID STATE "F MAS NMR STUDY OF OXYGEN/FLUORINE ORDERING IN OXYFLUORIDES, Lin-Shu Du, Francis Wang and C.P. Grey, SUNY at Stony Brook, Department of Chemistry, Stony Brook, NY 11794-3400.
- 10. THE USE OF THE INADEQUATE EXPERIMENT TO OBTAIN THROUGH-BOND CONNECTIVITIES IN SOLIDS, A. Lesage, C. Auger, S. Caldarelli and L. Emsley, Ecole Normale Superieure de Lyon, 69364 Lyon, France.
- MECHANISTIC STUDIES OF HIGH FREQUENCY DYNAMIC NUCLEAR POLARIZATION: 140 GHZ PULSED EPR AND ELDOR INVESTIGATIONS OF ELECTRON CROSS RELAXATION, C.T. Farrar. D.A. Hall, G.J. Gerfen, S.J. Inati, M.L. Bennati, and R. G. Griffin, Francis Bitter Magnet Lab, Massachusetts Institute of Technology 150 Albany Street, Bldg. NW14-4107 Cambridge, MA 02139.
- 12. TRIPLE, QUINTUPLE AND HIGHER ORDER MULTIPLE QUANTUM MAS NMR OF QUADRUPOLAR NUCLEI, C. Fernandez, J.-P. Amoreux, L. Delevoye, and M. Pruski, 1-CNRS URA801, Universite des Sciences et Technologies de Lille, 59655 Villeneuve d'Ascq, France; Ames Laboratory, Iowa State University Ames, Iowa 50011.
- 13. OXYGEN-17 NMR 1D AND 2D CHARACTERIZATION OF YTTRIUM OXYDE POLYMORPHS, P. Florian. D. Massiot, J.P. Coutures and P.J. Grandinetti, CNRS-CRPHT, 1D Av. Rech. Scientifique, 45071 ORLEANS CEDEX 2, France; Ohio State University, 120 W. 18th Avenue, Columbus OH 43210-1173.
- 14. TIME RESOLVED VERY HIGH TEMPERATURE NMR (UP TO 2400°C): INVESTIGATION OF THE STRUCTURE AND DYNAMICS OF HIGH TEMPERATURE LIQUIDS AND LIQUID-SOLID TRANSITION, <u>P. Florian</u>. D. Massiot, B. Touzo, D. Trumeau, V. Montouillout and J.P. Coutures, CRPHT-CNRS, 1D Av. Rech. Scientifique, 45071 Orleans Cedex 2, France.
- 15. SOLID-STA TE NMR INVESTIGATION OF "C AND "N LABELED NUCLEOSIDES AND NUCLEIC ACIDS USING DRAWS, <u>K. B. Geahigan</u>, J. M. Miller, S. S. Kiihne and G. P. Drobny, University of Washington, Department of Chemistry, Seattle, WA 98195.
- 16. VARIABLE TEMPERATURE LI-7 NMR STUDIES OF NICKEL SUBSTITUTED LITHIUM MANGANESE OXIDE SPINELS, <u>B.A. Gee</u>, C. Horne, E. Cairns and J.A. Reimer, Energy and Environment Division, Lawrence Berkeley National Laboratory, Department of Chemical Engineering, 201 Gilman Hall, University of California, Berkeley, CA. 94720.
- RELATIONSHIPS BETWEEN 0-17 NMR PARAMETERS AND STRUCTURE IN NETWORK-MODIFIED SILICATES AND THEIR APPLICATION TO GLASS STRUCTURE, P. J. Grandinetti. K. E. Vermillion, P. A. Florian, I. Farnan and J. F. Stebbins, Department of Chemistry, Ohio State University, Columbus, OH 43210, ; CRPHT, CNRS, 45071 Orleans, France; Department of Earth Sciences, Cambridge University, Cambridge CB2 3EQ, UK; Department of Geology, Stanford University, Stanford, CA 94305-2115.
- MRM CHARACTERIZATION OF MATERIALS USING GASEOUS AND LIQUID PROBES, <u>P.M.</u> <u>Gregory</u>. R. Gerald & RE. Botto, Chemistry Division, Argonne Ntional Laboratory, 9700 South Cass Ave., Argonne, IL 60439.
- 19. HEXAKIS(TRIFLUOROMETHYL)BENZENE IS NOT A SUITABLE "F- "C CROSS POLARIZATION STANDARD, <u>E.W. Hagaman</u> and D.K. Murray, Oak Ridge National Laboratory, P. O. Box 2008, Oak Ridge, Tennessee 37831-6201.
- 20. HIGH FREQUENCY (140 GHZ) ROTA TING FRAME DYNAMIC NUCLEAR POLARIZATION (RF-DNP), D.A. Hall. G.J. Gerfen, C.T. Farrar, S.J. Inati, M.L. Bennati and R.G. Griffin, Francis Bitter Magnet Lab, Massachusetts Institute of Technology, 150 Albany St., Bldg. NW14-4107, Cambridge, MA 02139.

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- 21. MAS NMR STUDIES OF CARBOTHERMAL SYNTHESIS OF LOW-Z BETA'-SIALON, K.J.D. MacKenzie, T. Ekstrom, G. V. White, and J.S. Hartman, New Zealand Institute for Industrial Research and Development, Lower Hutt, New Zealand; Department of Inorganic Chemistry, Stockholm University, Stockholm, Sweden; Department of Chemistry, Brock University, St. Catharines, Ontario L2S 3A1, Canada.
- 22. LI-7 AND DOUBLE RESONANCE NMR OF LITHIUM-INTERCALATED MICROPOROUS CARBONS, S.E. Haves, W.R. Even, R.W. Crocker, Zhengming Zhang and H. Eckert, Department of Chemistry, University of California, Santa Barbara, CA 93106; Sandia National Laboratories, P.O. Box 969, Livermore, CA 94551; Eveready Battery CO., P.O. Box 45077, Westlake, OH 44145.
- 23. *'LI NMR SINGLE CRYSTAL STUDY OF ALANYLGLYCINE LITHIUM BROMIDE DIHYDRATE, A.* Metz, <u>B. Herreros</u> and G.S. Harbison, Dept. of Chemistry, University of Nebraska at Lincoln, Lincoln, NE 68588-0304.
- 24. EXAMINATION OF DEFECT-ASSISTED DIFFUSION PROCESSES IN THE NL, AL, SYSTEM VIA "AL NMR AND POSITRON ANNHILATION SPECTROSCOPY, T. J. Bastow, G. W. West, A. J. Hill. M. E. Smith, A. Siegle and S. Koch, CSIRO Division of Materials Science and Technology, Private Bag 33, S. Clayton MDC, Clayton, VIC 3169 Australia; Dept. of Physics, University of Kent, Canterbury, Kent, UK CT2 7NR; Max-Planck-Institut fur Metallforschung, Postfach 80 06 65, 70506 Stuttgart, Germany.
- 25.
   CONFORMATIONAL MOTIONS WITHIN MOLECULAR CRYSTALS BY NMR RELAXATION,
   S. A.

   Holmes
   and J. H. Strange, Physics Laboratory, University of Kent, Canterbury, Kent, CT2 7NR, UK.
- 26. DYNAMIC NUCLEAR POLARIZATION IN DOPED BENZAMIDE AND DIBENZOFURAN, Jian Zhi Hu. Baolian Yang, R.A. Wind, D.M. Grant, R. J. Pugmire and Chaohui Ye, University of Utah, Pacific Northwest National Laboratory, and the Wuhan Institute of Physics, Wuhan, PRC.
- 27. NEW TECHNIQUES FOR NMR STUDIES OF HETEROGENEOUS CATALYSIS, P.K. Isbester. J. Grenz and E.J. Munson, University of Minnesota, 207 Pleasent St. S.E., Minneapolis, MN 55455.
- 28. WHAT CAN NMR AND IR SPECTROSCOPY TELL ABOUT THE PNA+SENSITIVITY OF ELECTRODE GLASSES, K. Herzog, B. Thomas, C. Jager, University of Mining and Technology, Institute of Analytical Chemistry, Leipziger Str. 29, 09596 Freiberg/Sa., Germany; Friedrich Schiller University, PATF, Max Wien Platz 1, 07743 Jena, Germany.
- 29. <sup>™</sup>XE NMR STUDIES OF COMPETITIVE ADSORPTION, <u>A.K. Jameson.</u> C. Jameson and P. Kostikin, Department of Chemistry, University of Illinois at Chicago 60607-7061; Loyola University, Chicago IL 60626.
- 30. GCMC SIMULATIONS OF THE "XE NMR CHEMICAL SHIFTS IN CAA, SILICALITE, AND FAUJASITES, C.A. Jameson, A.K. Jameson and Hyung-Mi Lim, Department of Chemistry, University of Illinois at Chicago 60607-7061; Loyola University, Chicago IL 60626.
- 31. SI-29 MAS NMR OF HIGHLY ORDERED POLYMER-SILICA NANOCOMPOSITES, Elizabeth Juang, Sanlin Hu, D.H. Gray, Doug Gin, J.A. Reimer, Materials Science Division Lawrence Berkeley National Laboratory and Depts. of Chemistry and Chemical Engineering, University of California, Berkeley, CA 94720.
- 32. INEPT EXPERIMENTS INVOLVING QUADRUPOLAR NUCLEI IN SOLIDS, <u>Hsien-Ming Rao</u> and C.P. Grey, Chemistry Department, State University of New York, Stony Brook, NY 17790-3400.
- 33. " C NMR SPECTRAL EDITING AND SPIN COUNTING ON THE ORGANIC COMPONENTS OF SOIL, D. Keeler and G.E. Maciel, Department of Chemistry, Colorado State University, Fort Collins, CO 80523.
- 34. A SOLID-STATE COBAL T-59 NMR STUDY OF OCTAHEDRAL COBALT(III) COMPLEXES, C.W. Kirby and W.P. Power. Guelph-Waterloo Centre for Graduate Work in Chemistry, Department of Chemistry, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada.
- 35. A MULTINUCLEAR SOLID STATE NMR STUDY OF COPPER(I) CYANIDE COMPLEXES, <u>S. Kroeker</u> and R.E. Wasylishen, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, B3H 4J3, Canada, and John Hanna, CSIRO North Ryde NMR Laboratory, P.O. Box 52, North Ryde, N.S. W. 2113, Australia.
- 36. DETERMINATION OF "SI CHEMICAL SHIFT TENSORS BY 2D-ROTOR SYNCHRONIZED MAS NMR ON SINGLE CRYSTALS. G.H. Kunath-Fandrei. H. Rager and C. Jaeger, Institute for Optics and Quantum Electronics, Friedrich-Schiller-University Jena, D-07743 Jena, Germany; Dept. Geol. Sci., University of Marburg, Hans-Meerwein-Strasse, D-35032 Marburg, Germany.
- 37. CALCULATING QUADRUPOLE COUPLING CONSTANTS, Young-Sik Kye and G.S. Harbison, Dept. of Chemistry, University of Nebraska, Lincoln, NE 68588-0304.
- 38. UBIQUITIN UNFOLDING THERMODYNAMICS AS PROBED BY HYDROGEN EXCHANGE, <u>H. Le.</u> M. Schick and R. R. Ernst, Labor, fur Physikalische Chemie, ETH-Zentrum, 8092 Zurich, Switzerland.
- 39. VARIABLE TEMPERATURE SOLID STATE NMR STUDIES OF THE BRONSTED ACID SITES OF HZSM-5 AND HSAPO-34, Haiming Liu, Hsien-Ming Kao and C.P. Grey, Department of Chemistry, State University of New York at Stony Brook, NY 11794-3400.
- 40. ON THE ORIGIN OF SPINNING SIDEBANDS IN MQMAS EXPERIMENTS, L. Marinelli and L. Frydman, Department of Chemistry (M/C 111), University of Illinois at Chicago, 845 W. Taylor Street, Chicago, IL 60607-7061.

https://digitalcommons.du.edu/rockychem/vol39/iss1/1 DOI: https://doi.org/10.56902/RMCMR.1997.39.1

- 41. THE STUDY OF A SERIES OF ORGANIC MOLECULES USING TPPM AND TIGER WITH "C PHORMAT SPECTRA, <u>G. McGeorge</u>, J. Harper, D. W. Alderman and D.M. Grant, University of Utah, Salt Lake City, Utah, 84112.
- \*XE AND ' H NMR STUDIES OF POLYSTYRENE NANOGELS, K. J. McGrath. C.M. Roland, M. Antonietti and M. Neese, Code 6120, Naval Research Laboratory, Washington, DC 20375; MPI Kolloid und Grenzflachenforschung, Kantstr 55 D 14513 Teltow, Germany.
- 43. CHARACTERIZATION OF QUADRUPOLAR AND CHEMICAL SHIFT TENSORS BY 2D MULTIPLE-QUANTUM NMR SPECTROSCOPY, <u>A. Medek</u> and L. Frydman, Department of Chemistry (M/Cl 11), University of Illinois at Chicago, 845 W. Taylor St., Chicago, JL 60607-7061.
- 44. INVESTIGATION OF DECOUPLING AND DIPOLE RECOUPLING TECHNIQUES OF UNIFORMLY LABELED COMPOUNDS UNDER HIGH SPEED MAS, <u>A.K. Mehta.</u> B.A. Tounge, S.T. Burns, Xiaoling Wu and K.W. Zilm, Department of Chemistry, Yale University, New Haven CT 06511.
- 45. "F DOUBLE QUANTUM DRAWS OF THE DICKERSON DODECAMER, M.E. Merritt. J. Stringer, K. Geahigan and G. Drobny, University of Washington, Chemistry Department. Box 351700, Seattle, WA 98195.
- 46. STUDY OF THE TEMPERATURE DEPENDENCE OF RELAXATION TIMES FOR SEVERAL PARAMAGNETIC METALLOPORPHYRIN COMPLEXES, <u>K. I. Momot.</u> F. A. Walker, Department of Chemistry, University of Arizona, Tucson, AZ, 85721.
- 47. A THEORETICAL STUDY OF THE DIPOLAR AND SCALAR CONTRIBUTIONS FROM THE UNPAIRED ELECTRON TO 'H NMR RELAXATION RATES IN LOW-SPIN METALLOPORPHYRIN COMPLEXES. K. I. Momot. F. A. Walker, Department of Chemistry, University of Arizona, Tucson, Arizona, 85721.
- CHARACTERIZATION OF MGAL<sub>0</sub>4 PRECURSOR POWDERS PREPARED BY AQUEOUS ROUTES.
   "AL MAS, MQ-MAS AND "AL-H REDOR INVESTIGATIONS, V. Montouillout. D. Massiot, A. Douy, C. Magnenet and J. P. Coutures, CNRS-CRPHT 1D avenue de la Recherche Scientifique, 45071 Orleans cedex 2 France.
- 49. "SI MAS NMR CHARACTERIZATION OF PDMS-SILICA COMPOSITES, S. A. Myers and A. Nazeri, Naval Air Warfare Center, Chemistry and Materials Branch, Code 4B2300D, China Lake, CA 93555; Naval Research Laboratory, Composites and Ceramics Branch, Code 6374, Washington, DC 20375.
- 50. SOLID-STATE NMR STUDIES OF POLYMORPHISM IN PHARMACEUTICALS, <u>B.E. Padden</u>. M.T. Zell, E.J. Munson, Haijian Zhu, Jane Li and D.J.W. Grant, Departments of Chemistry and Pharmaceutics, University of Minnesota, Minneapolis, MN, 55455.
- 57. DIRECT ASSIGNMENT OF 13C NMR SPECTRA OF RIGID SOLIDS BY TWO-DIMENSIONAL MAGIC ANGLE SPINNING SEPARATED LOCAL FIELD SPECTROSCOPY, Honghm Pan. Department of Chemistry, Texas A&M University, College Station, TX 77843-3255.
- 52. SOLID-STA TE NMR STUDIES OF POLYMER ORDER AND MOBILITY IN POLYMER-OXIDE NANOCOMPOSITES, W.P. Power, G.R. Goward, T.A. Kerr and L. F. Nazar, Guelph-Waterloo Centre for Graduate Work in Chemistry, Department of Chemistry, University of Waterloo, Waterloo, ON, N2L 3G1, Canada.
- 53. NIOBIUM-93 NUTATION SPECTROSCOPIC STUDY OF PIEZOELECTRIC LEAD MAGNESIUM NIOBATE AND RELATED MATERIALS, <u>S. Prasad</u>, P. Zhao, J. Huang, J.J. Fitzgerald and J. Shore, Department of Chemistry and Biochemistry, South Dakota State University, Brookings, SD 57007.
- 54. INVESTIGATION OF THERMAL TRANSFORMATIONS OF CLAY MINERALS BY AL AND "SI SOLID-STATE NMR, <u>G. Roch</u>, M.E. Smith and S. Drachman, Physics Laboratory, University of Kent, Canterbury, Kent, CT2 7NR, UK.; Redland Centre of Technology, Gatwick Road, Crawley, West Sussex, RH10 2NG, UK.
- 55. INVESTIGATIONS OF THE STRUCTURE AND "INTERFACIAL" SURFACE CHEMISTRY OF BIOGLASS BY SOLID-STATE MULTINUCLEAR NMR SPECTROSCOPY, <u>G. Sarkar</u> and John J. Fitzgerald, Department of Chemistry and Biochemistry, South Dakota State University, Brookings SD.
- 56. NMR INVESTIGATIONS ON RARE EARTH ALUMINOSILICATE GLASSES, <u>T. Schaller</u> and J.F. Stebbins, Department of Geological and Environmental Sciences, Stanford University, Stanford, California 94305-2115.
- 57. SURFACE NMR BY SPINOE OF LASER-POLARIZED XENON UNDER CONTINUOUS FLOW CONDITIONS, <u>R.</u> Scydoux. M. Haake, E. Brunner, J.A. Reimer and A. Pines, Materials Sciences Division, Lawrence Berkeley National Laboratory and the Departments of Chemistry and Chemical Engineering, University of California, Berkeley, CA 94720.
- 58. CHANGES IN THE STRUCTURE OF TSAREGORODTSEVITE [N(CH<sub>2</sub>),J[SI<sub>3</sub>(SI<sub>2</sub>AL,J06J<sub>2</sub> ON ANNEALING, <u>B.L. Sherriff</u>. G. Kunath-Fandrei, C. Jager, E. V. Sokolova, Dept. Geological Sciences, University of Manitoba, Winnipeg, Manitoba, Canada R3T 2N2; Institut fur Optik and Quantenoptik, Friedrich Schiller Universitat, Max-Wien Platz 1, D-07743 Jena, Germany; Dept. Crystallography, Faculty of Geology, Moscow State University, Moscow 119899, Russia.

- 59. CHARACTERIZATION OF MATERIALS USING MULTIPLE QUANTUM AND FIELD SWEEP NMR OF QUADRUPOLE NUCLEI, I.J.F. Poplett, <u>M.E. Smith and E.R.H. van Eck</u>, Department of Physics, University of Kent, Canterbury, Kent, U.K. CT2 7NR.
- THE APPLICATION OF TIME-DEPENDENT NMR DIFFUSION MEASUREMENTS FOR CHARACTERIZING POROUS MEDIA, C. H. Sotak, K. G. Helmer, M. D. Hurlimann, T. M. de Swiet, and P. N. Sen, Dept. of Biomedical Engineering, Worcester Polytechnic Institute, Worcester, MA 01609; Schlumberger-Doll Research, Ridgefield, CT 06877; Dept. of Chemistry, UC Berkeley, Berkeley, CA 94720.
- 61. *MEASUREMENT OF FLUORINE INTERNUCLEAR DISTANCES IN DNA AND RNA*, <u>J.A. Stringer</u>. J. Orban and G.P. Drobny, University of Washington, Chemistry Department BG-10, Seattle, WA 98195-0001.
- 62. FAST FIELD-CYCLING NMR STUDY OF MEMBRANE UNDULATIONS, J.O. Struppe. G. Klose and F. Noack, Universitaet Stuttgart, 70550 Stuttgart, Germany; Dept. of Chemistry, University of California San Diego, 9500 Gilman Drive, CA. 92093-0359; Physikalisches Institut, Universitaet Leipzig, 04103 Leipzig, Germany.
- 63. SOLUTION STRUCTURES OF LARIAT ETHERS AND THEIR ALKALI METAL SALTS BY NMR SPECTROSCOPY, <u>V.S. Talanov</u>, D. W. Purkiss and R. A. Bartsch, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX. 79409.
- 64. ULMS MICROPOROUS ALUMINO-PHOSPHATE. A P-31 NMR DOUBLE QUANTUM CHECK FOR SPATIAL GROUP DETERMINATION, <u>F. Taulelle.</u> C. Jager, T. Loiseau, J. Renaudin, G. Ferey, RMN et Chimie du Solide, UMR 50 CNRS, University Louis Pasteur, 4 rue Blaise Pascal, 67070 Strasbourg Cedex, France; Friedrich Schiller University, PATF, Max Wien Platz 1, 07743 Jena, Germany; IREM, UMR C 0173 CNRS, Institut Lavoisier; Universite de Versailles Saint Quentin, 45 avenue des Etats Unis 78035 Versailles, France; Laboratoire des Fluorures, ESA 6010 CNRS, Universite du Mans, 72017 Le Mans Cedex, France.
- 65. ARGYRODITES FAMILY. SYMMETRY ELEMENTS COUNTING BY NMR INEQUIVALENCE DETERMINATION AND PHASE TRANSITIONS STUDIES, <u>F. Taulelle</u>, E. Gaudin, M. Evain and C. Jager, RMN et Chimie du Solide, UMR 50 CNRS, Universite Louis Pasteur, 4 Rue Blaise Pascal, 67070 Strasbourg Cedex, France; Institut des Materiaux de Nantes, UMR 6502 CNRS, Universite de Nantes, 2 Rue de la Houssiniere, 44072 NANTES Cedex 03, France; Friedrich Schiller University, PATF, Max Wien Platz 1, 07743 Jena, Germany.
- 66. ANALYSIS OF MULTIPLE PULSE SEQUENCES FOR THE HIGH RESOLUTION OF SOLID-STATE NMR SPECTROSCOPY, D. Taylor. M.R. Kumar and A. Ramamoorthy, Biophysics Research Division and the Department of Chemistry, The University of Michigan, Ann Arbor, MI 48105.
- 67. HIGH FIELD CP MAS OF FULLY "C LABELED POLYCRYSTALLINE COMPOUNDS, <u>B.A.</u> Tounge, A.K. Mehta, Xiaoling Wu and K.W. Zilm, Department of Chemistry, Yale University New Haven, CT 06511.
- 68. <sup>III</sup>CD NMR CHARACTERIZATION OF CDS NANOCRYSTALLINE POWDERS OBTAINED BY PRECIPITATION FROM AQUEOUS SOLUTION, V. Ladizhansky, G. Hodes and S. Vega. Chemical Physics Department and Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, 76100 Israel.
- 69. A HIGH RESOLUTION SOLID STATE "C NMR INVESTIGATION OF THE LOCAL CHAIN DYNAMICS OF COMPATIBLE BLENDS OF POLYSTYRENE AND POLY(VINYL METHYL ETHER), <u>T.A. Wagler</u>. P.L. Rinaldi, Chang D. Han and Hyunaee Chun, The University of Akron, Akron, OH., 44325-3601.
- 70. SOLID-STATE NMR STUDIES OF SELF-ASSEMBLED MONOLAYERS ON ORDERED MESOPOROUS SUPPORTS (SAMMS), Li-Qiong Wang. Jun Liu, Xiangdong Feng, G.E. Fryxell, and G.J. Exarhos, Pacific Northwest National Laboratories, Richland, WA 99352.
- 71. NMR STUDIES OF SOME EUTECTIC FORMING SOLID AMINO ACID DERIVATIVES, <u>Yulan Wang</u> and P. S. Belton, Institute of Food Research, Norwich Laboratory, Norwich Research Park, Colney, Norwich NR4 7UA. UK.
- 72. IN SITU VARIABLE-TEMPERATURE ONE AND TWO-DIMENSIONAL PROTON CRAMPS STUDIES OF PROTON SPIN-EXCHANGE IN COALS, Jincheng Xiong and G.E. Maciel, Department of Chemistry, Colorado State University, Fort Collins, CO 80523.
- 73. VARIABLE-TEMPERATURE DEUTERIUM NMR STUDIES OF TRIPHENYLMETHYL CATIONS ON EXTERNAL AND INTERNAL SURFACES OF ZEOLITE HY, Jincheng Xiong. Ting Tao and G.E. Maciel, Department of Chemistry, Colorado State University, Fort Collins, CO 80523.
- 74. NOVEL NANOCOMPOSITES: AN NMR PROBE OF DYNAMICS, <u>Doo-Kyung Yang</u> and D. Zax, Department of Chemistry, Baker Laboratory, Cornell University, Ithaca, NY 14853.
- 75. <sup>3</sup>H NMR LINESHAPE STUDIES OF LOCAL MOTION OF ORGANIC POLLUTANTS ADSORBED IN SOIL COMPONENTS, Jincheng Xiong, D. Keeler, Jane J. Yang and G.E. Maciel, Department of Chemistry, Colorado State University, Fort Collins, CO 80523.
- 76. LEAD-207 NMR SPECTROSCOPIC STUDY OF PIEZOELECTRIC LEAD MAGNESIUM NIOBATE AND RELATED MATERIALS, P. Zhao. S. Prasad, M. Benjamin, J. Huang, J. J. Fitzgerald and J. Shore, Department of Chemistry and Biochemistry, South Dakota State University, Brookings, SD 57007.

77.

3.30

# NMR STUDIES OF LYOTROPIC AND THERMOTROPIC LIQUID CRYSTALLINE POLYMERS IN

**THEIR SOLID AND FLUID PHASES,** Min Zhou, V. Frydman, D. Mcelheny, and L. Frydman, Department of Chemistry (M/C 111), University of Illinois at Chicago, 845 W. Taylor Street, Chicago, IL 60607-7061.

#### Session III, NMR of Macromolecules

Jeff Reimer, Presiding

#### POLYMERS OF SUBSTITUTED N-PHENYLNORBORNENE-5,6-DICARBOXIMIDE:

CHARACTERIZATION OF STRUCTURE AND DYNAMICS, J. R. Garbow. J. Asrar and J. Goetz, Monsanto Corporate Research, Monsanto Company, St. Louis, MO 63167; Monsanto Growth Enterprises, Monsanto Company, St. Louis, MO 63167; Department of Chemistry, Washington University, St. Louis, MO 6 3130.

 4:00 THE USE OF CHEMICAL SHIELDING TENSORS TO DETERMINE DIHEDRAL ANGLES IN PROTEINS IN THE SOLID STATE, J. Heller. D.D. Laws, S. Bush, H.M.L. Bitter, D.E. Wemmer, A. Pines, R.H. Havlin and E. Oldfield, Dept. of Chemistry, University of California, Berkeley, CA 94720; Structural Biology Division and Material Science Division, Lawrence Berkeley National Laboratory; Dept. of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL, 61801.

- 4:45 SHEAR FLOW OF LIQUID CRYSTALLINE POLYMERS, <u>C. Schmidt</u>. Institute for Macromolecular Chemistry, University of Freiburg, Sonnenstr. 5, D-79104 Freiburg, Germany.
- 5:15 **PROTON AND FLUORINE NMR OF NAFION/SILICA COMPOSITES,** <u>A. J. Vega</u>. M.A. Harmer, Qun Sun and W. E. Farneth, DuPont Central Research and Development, P.O. Box 80356, Wilmington, DE 19880-0356.

## Tuesday, August 5,1997

#### Session IV, Inorganic Materials Including Glasses

#### John Hanna, Presiding

- 8:30 NETWORK CONNECTIVITIES IN OXIDE GLASSES STUDIED BY MULTINUCLEAR SINGLE AND DOUBLE RESONANCE NMR SPECTROSCOPY, L. Zuchner, M. Bertmer, L. van Wullen, S. Kaczmarek, N. Machida and <u>H. Eckert</u>, Institut fur Physikalische Chemie, Westfalische Wilhelms-Universitat Minister, SchloBplatz 7, D48149 Minister.
- 9:00 **DQ NMR INVESTIGATIONS OF PHOSPHATE AND SILICATE GLASSES,** <u>C. Jager.</u> P. Hartmann, R. Witter, K. Herzog, B. Thomas, Friedrich Schiller University, PATF, Max Wien Platz 1, 07743 Jena, Germany; University of Mining and Technology, Institute of Analytical Chemistry, Leipziger Str. 49,09596 Freiberg/Sa., Germany.
- 9.30 STRUCTURAL INVESTIGATIONS OF PHOSPHATE AND RELATED GLASSES USING ONE- AND TWO-DIMENSIONAL HETERONUCLEAR CORRELATION NMR, K.T. Mueller. R. M. Wenslow, J.M. Egan, K. Fiske and S. Prabakar, Department of Chemistry, The Pennsylvania State University, 152 Davey Laboratory, University Park, PA 16802-6300.
- 10:00 Break
- 10:30 SOLID-STATE "O MAS AND "P 2D EXCHANGE NMR INVESTIGATIONS OF STRUCTURE AND CONNECTIVITY IN PHOSPHATE GLASSES, T.M. Alam and R.K. Brow, Sandia National Laboratories, Albuquerque, NM 87185.
- 11:00 SOLID-STATE NMR STUDIES OF HETERONUCLEAR SPIN-PAIRS IN TRANSITION METAL COMPOUNDS, <u>R.E. Wasylishen</u>, K. Eichele, R. Schurko, and S. Kroeker, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, B3H 4J3, Canada.
- 11.30 MIXED X-RAY/NMR STRUCTURAL DETERMINATIONS ON SOLIDS, <u>F. Taulelle</u>. E. Gaudm, M. Evain, C. Jager, T. Loiseau, J. Renaudin and G. Ferey. RMN et Chimie du Solide, UMR 50 CNRS, Universite Louis Pasteur, 4 rue Blaise Pascal, 67070 Strasbourg Cedex, France; Institut des Materiaux de Nantes, UMR 6502; CNRS, Universite de Nantes, 2 Rue d e la Houssiniere, 44072 NANTES Cedex 03, France; Friedrich Schiller University, PATF, Max Wien Platz 1, 07743 Jena, Germany; IREM, UMR C 0173 CNRS, Institut Lavoisier; Universite de Versailles Sai nt Quentin, 45 avenue des Etats Unis 78035 Versailles, France; Laboratoire des Fluorures, ESA 6010 CNRS, Universite du Mans, 72017 Le Mans Cedex, France.

Tuesday, August 5,1997 Session V, Poster Session B Robert Wind, Presiding 1:30-3:00 (Even-numbered posters will be presented. See Session II for complete lisitng.)

<sup>4:30</sup> Break

Session VI, Inorganic/Dynamics/MQ NMR

#### Jeff Reimer, Presiding

- THE USE OF VERY FAST "F MAS NMR TO STUDY DISORDERED FLUORIDES AND FLUORIDE-ION 3:30 CONDUCTION, C. P. Grey, F. Wang and Lin-Shu Du, State University of New York at Stony Brook Chemistry Department, Stony Brook, NY 11794-3400.
- 4:00 ULTRASLOW MOTION IN METALLIC GLASSES DETECTED BY SPIN ALIGNMENT ECHO OF SPIN-3/2 NUCLEI, Xiao-ping Tang, Yue Wu, Department of Physics and Astronomy, University of North Carolina, Chapel Hill, NC 27599-3255.

4:30 Break

- APPLICATION OF SOLID STATE NMR TO TRANSITION METAL ALUMINIDE CHARACTERIZATION: 4:45 "AL, "SC, """TI, "V, "NI, "ZR, T.J. Bastow. M.A. Gibson and C.T. Forwood, Materials Characterisation Group, CSIRO Div Mat Sci & Tech, Private Bag 33, S. Clayton MDC, Clayton, VIC 3169 Australia.
- **GROWTH OF MULTIPLE-OUANTUM NMR COHERENCES IN SOLIDS,** 5:15 A.K. Khitrin. Institute of Chemical Physics, Chernogolovka, Moscow reg., 142432 Russia.

#### **Tuesday Evening, August 5,1997**

7:30-9:00 p.m.

Session VII, Vendor Poster Session **Robert Wind, Presiding** 

## Wednesday, August 6,1997

#### Session VIII, Robert W. Vaughan Memorial Session

- 8:30 R.W. VAUGHAN PLENARY LECTURE: PROBING SUPERCONDUCTIVITY BY NMR, Charles P. Slichter, Center for Advanced Study Professor of Physics and Chemistry, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, IL 61801-3080.
- NMR DOUBLE RESONANCE PROBES OF STRUCTURAL DISTORTIONS IN ALKALI FULLERIDE 9.30 SUPERCONDUCTORS, K. Gorny, C. Hahm, J.A. Martindale, C.H. Pennington. D.R. Buffinger and R. P. Ziebarth, Department of Physics, Ohio State University; 174 W. 18th Avenue; Columbus, Ohio 43210. 10:10 Break
- 10:40 OPTICAL PUMPING FOR APPLICATIONS IN BIOMOLECULAR SOLID STATE NMR, R. Tvcko. National Institutes of Health Building 5, Room 112 Bethesda, Maryland 20892-0520.

CHAIN PACKING AND DYNAMICS IN PURE POLYCARBONATE AND POLYCARBONATE 11:20 COPOLYMERS, CA. Klug. D. H. Whitney, R. Yaris, J. Wu, A.F. Yee and J. Schaefer, Department of Chemistry, Washington University, St. Louis, MO 63130; Department of Materials Science and Engineering, The University of Michigan, Ann Arbor, MI 48109.

#### Wednesday, August 6,1997

#### Session IX, Spatially Resolved Dynamics and Structure

#### Steve Sinton, Presiding

- NMR IMAGING OF CONCENTRATED SUSPENSIONS, S.A. Altobelli. A. Caprihan and E. Fukushima, 1:30 Lovelace Institutes, 2425 Ridgecrest, SE, Albuquerque, NM 87108.
- 2:00 3D - VISUALISATION AND QUANTITATION OF COMPLEX FLOW BY MAGNETIC RESONANCE IMAGING, L.D. Hall, A. Hanlon, S.G. Gibbs, D Haycock, S. Ablett and W. Frith, Herschel Smith Laboratory for Medicinal Chemistry, University of Cambridge School for Clinical Medicine, Robinson Way, Cambridge CB2 2PZ, UK; Unilever Research Colworth Laboratory, Colworth House, Sharnbrook, Bedford MK44 1LQ.
- PGSE NMR MEASUREMENTS OF TAYLOR VORTICES IN CONCENTRIC AND ECCENTRIC 2.30 CYLINDERS, J.P. Seymour. S. A. Altobelli, P.T. Callaghan, E. Fukushima and B. Manz, The Lovelace Institutes, 2425 Ridgecrest Dr. SE, Albuquerque, NM 87108; Dept. of Physics, Massey University, Palmerston North, New Zealand; Dept. of Chemical Engineering, Cambridge University, UK. Break
- 3:00

#### Session X, Optically-Pumped Xenon NMR, Surfaces and Zeolites

#### Steve Sinton, Presiding

A NEWPROBE FOR SURFACES: MULTIPLE-QUANTUM FILTERED GAS-PHASE XENON-131 NMR, 3:30 T. Meersmann. S. A. Smith and G. Bodenhausen, National High Magnetic Field Laboratory 1800 E. Paul Dirac Dr., Tallahassee, Fl 32310; Departement de Chimie, Ecole Normale Superieure, 24 rue Lhomond 75231 Paris Cedex 05, France.

- 4:00 **CIRCULATING LASER-POLARIZED XENON: STEADY-STATE HIGH SPIN POLARIZATION FOR** NMR, M. Haake, R. Seydoux, J. A. Reimer and A. Pines, Materials Science Division, Lawrence Berkeley Laboratory and the Departments of Chemistry and Chemical Engineering, University of California, Berkeley, CA 94720.
- 4:30 Break
- 4:45 <sup>19</sup>XE NMR OF OPTICALLY POLARIZED (OP) XENON ON THE SURFACES OF ICE AND CLATHRATE HYDRATES, <u>I.L. Moudrakovski</u>. C.I. Ratcliffe, J.A. Ripmeester, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada.
- 5:15 "O NMR OF ZEOLITES, L.M. Bull, R. Dupree and A. Samoson, Institut des Materiaux de Nantes, 2 Rue de la Houssinere, Nantes 44322 France; Department of Physics, University of Warwick, Coventry CV4 7AL, U.K.; Institute of Chemical Physics and Biophysics, Akadeemia Tee 23, Tallinn, EE0026, Estonia.

#### Thursday, August 7,1997

#### Session XI, Multi-Dimensional and Multiple-Quantum NMR: Lucio Frydman, presiding

- 8:30 ORDER-RESOLVED SIDEBAND SEPARATION IN MAGIC ANGLE SPINNING NMR OF HALF INTEGER QUADRUPOLAR NUCLEI, D. Massiot, V. Montouillout, F. Fayon, <u>P. Florian</u> and C. Bessada, CRPHT-CNRS, 1D Av. Rech. Scientifique, 45071 Orleans cedex 2, France.
- 9:00 MULTIPLE-QUANTUM MAS-NMR WITH CROSS-POLARIZATION, M. Pruski. D.P. Lang, C. Fernandez, L. Delevoye and J.P. Amoureux, Ames Laboratory, Iowa State University, Ames, IA 50011,; Laboratoire de Dynamique et Structure des Materiaux Moleculaires, CNRS URA 801, 59655 Villeneuve d'Ascq Cedex, France.
   9 30 ENHANCED NUCLEAR SPIN DIFFUSION BY SLOW MAGIC-ANGLE SAMPLE SPINNING FOR THE

*EXPLORATION OF SOLIDS,* <u>Zhehong Gan.</u> P. Robyr and R. R. Ernst, Laboratorium fur Physikalische Chemie, ETH-Zentrum, 8092 Zurich, Switzerland.

- 10:00 Break
- 10:30 TECHNIQUE FOR IMPORTING GREATER EVOLUTION RESOLUTION INTO "C PHORMAT SPECTRA, D.M. Grant. D. W. Alderman, R.J. Pugmire, G. McGeorge and J. Harper, University of Utah, Salt Lake City, UT, 84112.
- 11:00 MULTI-DIMENSIONAL CORRELATION EXPERIMENTS FOR THE MEASUREMENT OF DIPOLAR AND QUADRUPOLAR COUPLINGS IN SOLID-STATE NMR, L. Emsley. Ecole Normale Superieure de Lyon, 69364 Lyon, France.
- 1130SOLID-STA TE NMR STRUCTURE DETERMINATION OF ORIENTED PROTEINS, S.J. Opella.Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104.
- 12:00 Concluding Remarks, James Yesinowski

# SYMPOSIUM ON PHARMACEUTICAL ANALYSIS

Organized by Michael Cutrera, Robert K. Lantz, and Patricia L. Sulik

## Tuesday, August 5, 1997:

#### Robert K. Lantz, presiding

9:45	ISO 9001 VALIDATION, Glen Emelock. CRO Group, Melrose, MA.
10:45	Break
11:00	VALIDATION OF FT/IR SPECTROMETER FOR PHARMACEUTICAL APPLICATIONS, S. Bouffard.
	Perkin Elmer, San Jose, CA.

#### Wednesday, August 6,1997:

#### Morning Session: Michael Cutrera, presiding, Mac-Mod® Analytical Open Forum III

- 8:30 MODERNIZING HPLC METHODS I: ASSURING METHOD ROBUSTNESS, THINGS YOU MIGHT OVERLOOK
- 9:30 Break
  9:45 MODERNIZING HPLC METHODS II: UPGRADING CURRENT METHODS; IS THE GAIN WORTH THE PAIN?
- 10:45 Break
- 11:00 MODERNIZING HPLC METHODS III: LC/MS IS HERE TO STAY! SOME PRACTICAL ADVICE ON COLUMN AND MOBILE PHASE SELECTION.

#### Afternoon Session: Michael Cutrera, presiding

1:30 **CALIBRATING A UV/VIS SPECTROMETER - THE BEST APPROACH,** Adrea C. Reeves and Jerry D. Messman, SpectroStandards Analytical, Ft. Collins, CO.

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- 2:15 FAT OXIDATION IN RURAL GAMBIAN WOMEN, B.J. Sonko, P.W. Fennessey, Deptments of Pediatrics and Cardiology, UCHSC, Denver, CO.
- 2:35 AN ASSAY FOR AMIODARONE AND ITS METABOLITE DESMETHYLAMIDODARONE IN HUMAN PLASMA USING IONSPRAY TANDEM MASS SPECTROMETRY(LC/MS/MS), L.D. Winslow, D. Winburn, W, Martin, Kansas City Analytical Service, Shawnee, Kansas 66216.
- 2:55 *GC/MS OF HYDROXYL RADICAL FORMATION DURING CARDIAC INFARCT*, A.W. Pike, E. Kong, L Horowitz, P. Fennessey, Departments of Pediatrics and Cardiology, UCHSC, Denver, CO.

3:15 Break

3:30 HPLC METHOD DEVELOPMENT, R. Albrecht & Lloyd Snyder, LC Resources.

# SYMPOSIUM ON QUALITY ASSURANCE

Organized by Carl Craig

#### Tuesday, August 5,1997

#### Afternoon Session

- 1:20 **ROUTINE QC STANDARDS USED AS A GUIDE TO CONDUCTING DETECTION LIMIT STUDIES**, Larry Penfold and William Sullivan, Quanterra, Inc., 4955 Yarrow St., Arvada, CO 80020.
- 1:45 INDEPENDENT VALIDATION AND VERIFICATION TESTING OF TRACE EXPLOSIVE DETECTION SYSTEMS FOR ENHANCED AIR TRANSPORTATION SECURITY. David F. Glenn. David F. Gianotto, Carta J. Miller, Steven D. Hartenstein, LMITCO, INEEL, P.O. Box 1625-3840, Idaho Falls, ID 83415; Susan F. Hallowell, FAA, FAA Technical Center, AAR-520, Atlantic City IntT Airport, NJ 08405.
- 2:10 THE DEPARTMENT OF ENERGY'S INTEGRATED PERFORMANCE EVALUATION RPOGRAM (IPEP): PILOT STUDIES FOR IMPLEMENTATION. P. C. Lindahl. W.E. Streets, J.J. Marr, and K.J. Parish, Argonne National Laboratory, Argonne, IL 60439; W.R. Newberry, U.S. Department of Energy, Washington, DC 20585; J.R. Dahlgran, U.S. Department of Energy-, Idaho Falls, ID 83415; C. Watkins and J. Connolly, Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID 83415; and J. Fisk and L. A. Souza, Los Alamos National Laboratory, Los Alamos, NM 87545
- 2:35 Break
- 2:55 ENVIRONMENTAL REFERENCE MATERIALS ISSUES AND PERSPECTIVES. Chuck Wibby. Environmental Resource Associates, 5540 Marshall St., Arvada, CO 80002
- 3:20 COMPARISON OF ORGANIZATION QUALITY ASSURANCE REQUIREMENTS. Jerry Parr. Quanterra, Inc., 4955 Yarrow St., Arvada, CO 80020

# SYMPOSIUM ON RADIOCHEMISTRY

Organized by Ann Mullin

#### Monday, August 4,1997

#### Morning session: Ann Mullin, presiding

- 8:10 Welcoming Remarks, Ann Mullin, U.S. Geological Survey
- 8:15 **NATURALLY OCCURRING RADON IN HYDROLOGIC STUDIES** Matthew L. Schirmer, and <u>Michael P. Neary</u>, Center for Applied Isotope Studies, University of Georgia, 120 Riverbend Road, Athens, GA 30605.
- 8:45 GROSS ALPHA ACTIVITY IN RADIUM BEARING GROUND WATER IN THE COASTAL PLAIN OF NEW JERSEY by Zoltan Szabo, U.S. Geological Survey, 810 Bear Tavern Road, Suite 206, West Trenton, NJ 08328.
- 9:15 **RADIOASSAY OF RADIUM ISOTOPES BY COINCIDENCE SPECTROMETRY David McCurdy.** Yankee Atomic Environmental Laboratory, 580 Main St., Bolton, MA 01740.
- 9:45 Break
- 10:00 CALIBRATION BIAS IN MEASUREMENT OF RA-226 IN SOILS BY GAMMA SPECTROMETRY Michael Goodwill. Paragon Analytics, Inc., 225 Commerce Dr., Fort Collins, CO 80524.
- 10:30PREPARATION OF CALIBRATED MIXED, LONG-LIVED RADIONUCLIDE SOURCE FOR ALPHA<br/>SPECTROSCOPY Dr. Carter Hull. Oxford Instruments, 601 Oak Ridge Turnpike, Oak Ridge, TN 37831-2560.
- 11 00 TEMPORAL CHANGES OF SELECTED RADIOCHEMICAL CONCENTRATIONS IN GROUND WATER AT THE IDAHO NATIONAL ENGINEERING LABORATORY, IDAHO Roy C. Bartholomay, and Leroy L. Knobel, U.S. Geological Survey, INEL, Ms 4148, P.O. Box 2230, Idaho Falls, ID 83403.

30

11:30 USE OF THE "METHOD DETECTION LIMIT" VERSUS "MINIMUM DETECTABLE CONCENTRATION" IN THE MEASUREMENT AND REPORTING OF TRITIUM IN AQUEOUS SILICA GEL DISTILLATES Robert Shannon, Paragon Analytics, Inc., 225 Commerce Dr., Fort Collins, CO 80524.

Afternoon session: Tom Maloney, presiding

- 1:30 A NEW TOOL IN THE EVALUATION OF GAMMA-RAY SPECTRAL ANALYSIS SOFTWARE D.<u>R</u> Porterfield.
   G.H. Brooks, Jr., S.R Garcia, Y.O. Giles, N.L. Koski, and B.L. Lockhart, Los Alamos National Laboratory, P.O. Box 1663, MSK 484, CST-3, Los Alamos, N.M. 87545.
- 2:00 AUTORAMP AN AUTOMATIC UNIT FOR UNATTENDED AEROSOL COLLECTION, GAMMA-RAY ANALYSIS AND DATA TRANSMISSION FROM REMOTE LOCATIONS Colin Sanderson. Norman Latner, Vincent Negro, Scott Wurms, and Norman Chiu, U.S. Department of Energy, Environmental Measurements Laboratory, 201 Varick St., New York, NY 10014-4811.
- 2.30. **MEASUREMENT OF FLUORESCENCE FROM LOW CONCENTRATIONS OF DNA USING GAMMA RADIATION AS AN EXCITATION SOURCE** Michael P. Neary. and Richard N. Winn, Center for Applied Isotope Studies, University of Georgia, 120 Riverbend Road, Athens, GA 30605.

3:00 Break

- 3:15 ANALYSIS OF PB-210 IN WATER AND SOIL SAMPLES USING EICHROM'S LEAD RESIN Anil Thakkar. and Dr. James Harvey, EICHROM Industries, Inc., 8205 S. Cass Ave. #107. Darien, IL 60561.
- 3:45 NP-237 SEPARATION AND PURIFICATION BY ANION EXCHANGE CHROMATOGRAPHY Antony M.V. Vargees. and Robert Shannon, Paragon Analytics, Inc., 225 Commerce Dr., Fort Collins, CO 80524.

## Tuesday, August 5,1997

#### Morning session: Catherine Klusek, presiding

- 8:15 **OVERVIEW OF MARLAP** John Griggs. U.S. Environmental Protection Agency, NAREL, 540 South Morris Ave, Montgomery, AL 36115-2601.
- 8:45 QUALITY ASSESSMENT PROGRAM: PERFORMANCE EVALUATION FOR **ENVIRONMENTAL** RADIOCHEMISTRY **U.S.** DEPARTMENT 0F ENERGY, **ENVIRONMENTAL MEASUREMENTS** LABORATORY Pamela D. Greenlaw, and Catherine S. Klusek, USDOE Environmental Measurements Laboratory, 201 Varick St, New York, NY 10014-4811.
- 9:15 PROCESS CONTROL AND QUALITY ASSURANCE IN THE COMMERCIAL RADIOCHEMICAL LABORATORY, Lee Scott and Mathias Lardy, Quanterra, Inc, 2800 George Washington Way, Richland, WA 99352.
   9:45 Break
- 9:45
   Break

   10:00
   ARE MATRLX SPIKES COST EFFECTIVE FOR ENVIRONMENTAL RADIOCHEMICAL ANALYSES? Keith Wegner, Correlation Corporation, 300 Union Blvd., Suite 600, Lakewood, CO 80228, and Karen Schoendaller, Accu
- Labs Research, Inc., Golden, CO 80403-1650.
   10:30 STATISTICAL COMPARISON OF REPLICATE PAIRS OF SAMPLES COLLECTED FOR THE U.S. GEOLOGICAL SURVEY QUALITY ASSURANCE PROGRAM AT THE IDAHO NATIONAL ENGINEERING LABORATORY, IDAHO Leroy L. Knobel. Linda M. Williams, and Roy C. Bartholomay, U.S. Geological Survey, INEL, MS 4148, P.O. Box 2230, Idaho Falls, ID 83403.
- 11:00 *ILLUSTRATION OF LABORATORY QUALITY CONTROL CONCEPTS USING A SIMULATED ANALYSIS,* Jerry Parr and Lindsay Greyer. Quanterra Envirnomental Services, 4955 Yarrow St, Arvada, CO 80002.

## Afternoon session: John Griggs: presiding

- 1:30COMPARISON OFSENSITIVITYANDTHROUGHPUTFORALPHA/BETAMEASUREMENTSBrianCrandell, SRP, and Stan DeFilippis, Oxford Instruments, 601Oak Ridge Turnpike, Oak Ridge, TN37831-2560.
- 2:00 EFFICIENCY CORRECTION AS A FUNCTION OF INGROWTH FOR RA-116 DETERMINATION GAS FLOW PROPORTIONAL COUNTING David Burns, and Renee Gallegos, Paragon Analytics, Inc., 225 Commerce Dr, Fort Collins, CO 80524.
- 2:30 HYDROLOGICAL STUDIES BASED ON TRITIUM ANALYSIS TO ENRICH OR NOT TO ENRICH Michael P. Neary. Center for Applied Isotope Studies, University of Georgia, 120 Riverbend Road, Athens, GA 30605.
   3:00 Break
- 3:15 AN INNOVATIVE ENVIRONMENTAL DOWN-HOLE LOGGING MEASUREMENT SYSTEM USING SCINTILLATION DETECTORS Bill Richardson, Oxford Instruments, 601 Oak Ridge Turnpike, Oak Ridge, TN 37831-2560.
- 3:45 DETERMINATION OF WATERBOUND TRITIUM IN LOW MOISTURE SILICA GEL SAMPLES MICROWAVE DISTILLATION Bahman Pirastah, Paragon Analytics, Inc,. 225 Commerce Dr, Fort Collins, CO 80524.

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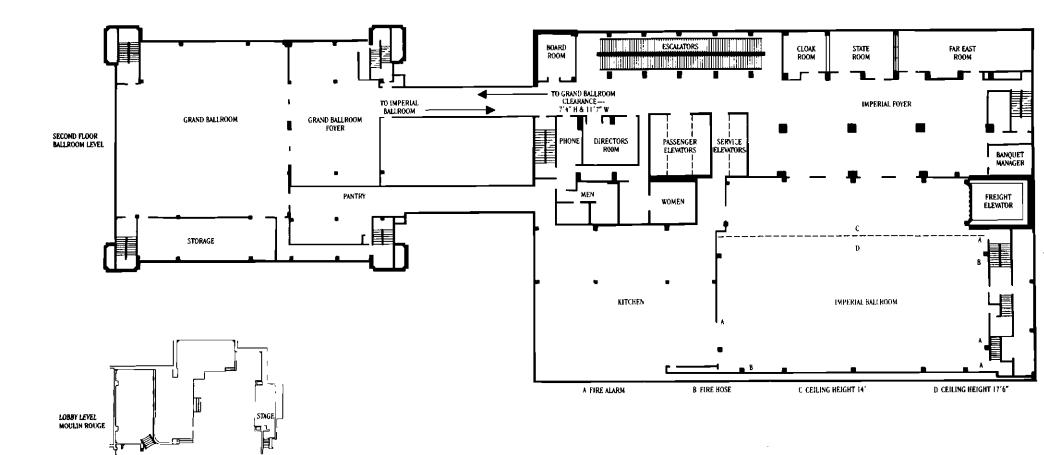
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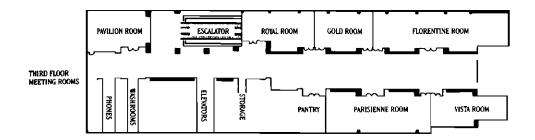
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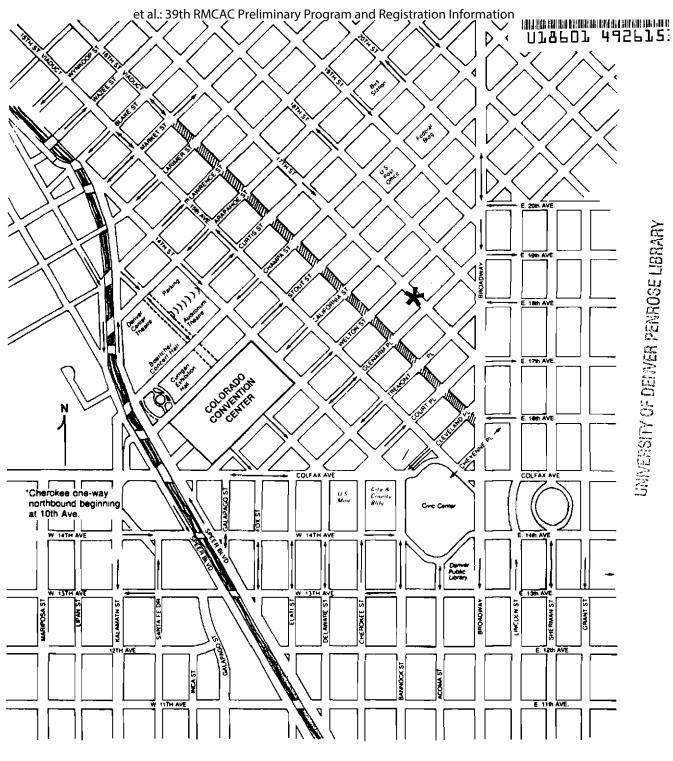
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