55th Annual Pentasectional Meeting of the American Chemical Society

Program and Abstracts
10 April 2010
Embassy Suites Hotel & Conference Center
Norman, OK
Map to Embassy Suites Hotel & Conference Center

Embassy Suites Hotel & Conference Center
2501 Conference Drive, Norman, OK
Tel: 405-364-8040
Fax: 405-364-3377
embassysuitesnorman.com

DIRECTIONS
From the North:
Exit Tecumseh Road, turn left.
Turn right on 24th Avenue NW.
Turn left on Conference Drive.

DIRECTIONS
From the South:
Exit Robinson Street, turn left.
Turn left on 24th Avenue NW.
Turn right on Conference Drive.
55th Annual Pentasectional Meeting of the American Chemical Society

Program and Abstracts
10 April 2010
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Norman, OK

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2010 Pentasectional Organizing Committee
(Chemistry and Biochemistry, The University of Oklahoma) Charles Rice – Conference Chairs
(Physics and Astronomy, The University of Oklahoma) Lloyd Bumm
(Chemistry and Biochemistry, Oklahoma State University) Nicholas Materer – Web Operations
Conference Venue Floor Plan

Embassy Suites Conference Center

Sooner A
Sooner B

Registration

G
H
I
J

Parking Lot

ENTRANCE

Breakfast and Coffee Breaks Served in the Exhibitor Area

Ballrooms

Lunch

A
B
C

to Hotel Lobby

[2]
### Conference Program Overview

<table>
<thead>
<tr>
<th>Time</th>
<th>University Ballroom A</th>
<th>University Ballroom B</th>
<th>University Ballroom C</th>
<th>Oklahoma Ballroom G</th>
<th>Oklahoma Ballroom H/I</th>
<th>Oklahoma Ballroom J</th>
<th>Sooner A</th>
<th>Sooner B</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:00 - 8:30 am</td>
<td>Nanotech Morning Session</td>
<td></td>
<td></td>
<td>NMR Spect.</td>
<td>Exhibits Open</td>
<td>NMR Spect.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8:30 - 10:00 am</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Biofuels Morning Session</td>
<td></td>
<td>X-Ray Crystal.</td>
<td>Chemical Education /POGIL</td>
</tr>
<tr>
<td>10:00 - 10:20 am</td>
<td>Break, refreshments in Ballroom H/I</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:20 - 11:40 am</td>
<td>Nanotech Morning Session</td>
<td></td>
<td></td>
<td>NMR Spect.</td>
<td>Exhibits Open</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11:40 - 12:00 am</td>
<td>Break, move to Ballroom B &amp; C for Lunch</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>12:00 - 12:40 pm</td>
<td>Lunch</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>12:40 - 1:00 pm</td>
<td>OK Chemist of the Year</td>
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<tr>
<td>1:00 - 2:00 pm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Poster Session</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2:00 - 3:30 pm</td>
<td>Nanotech Afternoon Session</td>
<td>Analytical and Physical Chemistry</td>
<td>Organic Chemistry</td>
<td>Biochem</td>
<td>Exhibits Open</td>
<td>Biofuels Afternoon Session</td>
<td>Future Planning Meeting</td>
<td></td>
</tr>
<tr>
<td>3:30 - 3:50 pm</td>
<td>Break -- refreshments in Ballroom H/I</td>
<td></td>
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</tr>
<tr>
<td>3:50 - 5:00 pm</td>
<td>Nanotech Afternoon Session</td>
<td>Analytical and Physical Chemistry</td>
<td>Pharm. &amp; Natural Products</td>
<td>Envir. &amp; Natural Products</td>
<td>Exhibits Open</td>
<td>Biofuels Afternoon Session</td>
<td>Inorganic Chemistry</td>
<td></td>
</tr>
<tr>
<td>5:00 - 6:00 pm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Vendor Take Down and Poster Removal</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>
Dr. Jiten Chatterji is the 2010 Oklahoma Chemist Awardee. He was born in India and graduated with a bachelor’s and master’s degree in chemistry from the University of Bihar. He attended the University of Wyoming and earned a Ph.D. in Physical Organic Chemistry under Dr. Rhodes in 1967. He was employed as a Developmental Chemist by Halliburton Energy Services and began working in the fracturing section starting on June 5, 1967. He retired from Halliburton as a Senior Scientific Advisor on December 31, 2009. This rank at retirement was the highest which Halliburton awards to its employees.

The major accomplishments in his last position included setting up drilling fluids; introduction of defoamers; high temperature fluid loss additives; biodegradable cement dispersants; high temperature stable cement foamers; salt tolerant latex systems; use of kiln dust to reduce the carbon footprint; non-dispersing high temperature cement retarders and lost circulation materials.

His impressive record of more than 176 active USA patents and 55 active foreign patents as well as his skills in oil field cementing are legendary. As one of his support letters indicated, Dr. Chatterji’s work on cement retarders and slurried cement retarders has led to millions of pounds being sold each year. The total volume of revenue and jobs created by this work is essentially unmeasurable. He has also played a major role in the development of hydraulic-fracturing technology which enables industry to operate marginal oil wells. He has been labeled as a superior leader by his colleagues at Halliburton and by others in companies which have utilized the technology which Dr. Chatterji created.
Past Recipients of the Oklahoma Chemist Award

<table>
<thead>
<tr>
<th>Year</th>
<th>Name</th>
<th>Year</th>
<th>Name</th>
<th>Year</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1973*</td>
<td>Otis C. Dermer</td>
<td>1986</td>
<td>Sherril D. Christian</td>
<td>2001</td>
<td>George R. Waller</td>
</tr>
<tr>
<td>1975</td>
<td>Charles M. Starks</td>
<td>1988</td>
<td>Marvin K. Kemp</td>
<td>2003</td>
<td>James Weaver</td>
</tr>
<tr>
<td>1979</td>
<td>Lionel M. Raff</td>
<td>1993</td>
<td>Bing M. Fung</td>
<td>2007</td>
<td>Ziad ElRassi</td>
</tr>
<tr>
<td>1981</td>
<td>Alfred Clark</td>
<td>1996</td>
<td>Max P. McDaniel</td>
<td>2009</td>
<td>Richard A. Bunce</td>
</tr>
<tr>
<td>1982</td>
<td>Marvin M. Johnson</td>
<td>1997</td>
<td>Donald L. Thompson</td>
<td>2010</td>
<td>Jiten Chatterji</td>
</tr>
<tr>
<td>1983</td>
<td>Simon Wender</td>
<td>1998</td>
<td>Roger E. Frech</td>
<td></td>
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<tr>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>* No award was given in 1972, 1991, and 1994.</td>
</tr>
</tbody>
</table>

The Oklahoma Chemist Award is sponsored by the five Oklahoma Sections of the American Chemical Society with the additional support of the chemical industries of the state of Oklahoma. We are grateful for the support. The recipient is the automatic nominee for the Southwest Chemist Award of the Southwest Region. Nominations for next year should be submitted to the local section representative of the Oklahoma Chemist Committee. The permanent committee chair is K. Darrell Berlin, Chemistry Department, Oklahoma State University, Stillwater, OK 74078.
Banquet Speaker

STEVE PARIS

In February 2003, Steve Paris rejoined the team at OCAST (the Oklahoma Center for the Advancement of Science and Technology) after nearly a four year break in service. In the interim, he served on the staff of the Oklahoma Technology Commercialization Center as the center’s director of marketing and as press secretary for the Brad Henry for Governor Campaign.

At OCAST, he is responsible for the agency’s public information program and the rural economic development initiative. He also is founder and co-host of Oklahoma Innovations, a statewide science weekly radio program heard each week on KRMG in Tulsa, KTOK in Oklahoma City and on stations served by Cameron University in Altus, Ardmore, Chickasha, Clinton, Duncan, Lawton/Ft. Sill, Woodward and Wichita Falls, Texas. The program is in its 15th year.

While at the Tech Center, he was responsible for the design, development, implementation and evaluation of the Tech Center’s strategic marketing plan and brings almost thirty years of experience in media relations, journalism and marketing management to the center’s management team. Prior to joining the Tech Center staff, Paris was Director of Technology Information for OCAST, the state’s science agency. He is also the past president of OPEA, the Oklahoma Public Employees’ Association.

Paris has served as the director of information services for the Oklahoma Tourism and Recreation Department and as director of the Information Division for the Oklahoma Farm Bureau, the state’s largest general farm organization. He was charter president of the Heartland Chapter, District Five, of OPEA and was the 1996 recipient of the OPEA Gaines Stout Award. Paris is a private pilot and served eight years in the Oklahoma Army National Guard.

A native of Muskogee, Oklahoma, Paris and his wife, Theresa make their home near Edmond. He is a graduate of Northeastern State University, Tahlequah, and while attending Northeastern, was a reporter for the Muskogee Phoenix. He has done postgraduate work at Oklahoma State University, Stillwater, Southern Illinois University in Carbondale and Oklahoma City University. Paris has served on the board of directors of the Oklahoma League for the Blind and as a co-chair of the Oklahoma Rural Development Council. He also serves as vice-president of the board of directors of Logan County Rural Water District No. 1.

In 2003, Paris was appointed by Governor Henry to serve on the Board of Trustees of the Oklahoma Public Employees Retirement System, a $6 billion retirement program that serves state employees and Oklahoma’s judges and justices.
Acknowledgements

We are extremely grateful to the following exhibitors for financial contributions and providing merchandise. Please visit the exhibitor area and thank them for their support of the American Chemical Society and the Oklahoma Pentasectional Meeting.

We would also like to express our gratitude to Embassy Suites, Tasha Houck, and staff, for their assistance with the conference arrangements.

- Department of Chemistry and Biochemistry
  The University of Oklahoma
- Department of Chemistry
  Oklahoma State University
- Graduate Programs at
  The University of Oklahoma Health Sciences Center
- McGraw-Hill Higher Education
- Buchi Corporation
- Ricca Chemical Company
- Pearson Education
- Kimble-Chase
- Wilmad-LabGlass
- Agilent Technologies
- Nikon Instruments
- Bruker BioSpin
- Mallinkrodt-Baker
- Rigaku
- Corning
As our department enters its second century we are preparing chemists and biochemists to meet the challenges of the next 100 years.

- Our award-winning graduate faculty of 29 chemists and biochemists has averaged nearly $10 million per year in external research funding over the past half dozen years. Faculty members have received honors including the Cottrell Teacher-Scholar Award, NIH First awards, a Guggenheim Fellowship, NSF-Career Awards, Alexander von Humboldt Scholar Awards and Fulbright Awards.

- Our award-winning students have been recognized with a NIH Graduate Fellowship, NSF Bridge to the Doctorate Fellowships, a Rhodes Scholarship, GAANN fellowships, University Alumni and President’s Fellowships. In recent years, an annual average of 12 Ph.D.’s and several MS degrees have been earned by our graduate students.

- New Research Building ($72 million, 160,000 sq. ft) completed in summer 2010.

- $22,000 departmental stipend. This is cash in your pocket. The cost of living in a “college town” like Norman is very low, so this stipend provides a comfortable lifestyle.

- Full Tuition Waver. You can enroll for research credit hours (in addition to course work credits) during the fall/spring and summer which will help you meet the minimum graduation hours very quickly. Thus, you can quickly reach the 90 credit hours required for graduation, perhaps in 4 years. 90/4 = 22.5 hrs/year, which is met with 8 hrs in the Fall (2 classes @ 3 hrs each + 2 research hours), 8 hrs in the Spring (2 classes @ 3 hrs each + 2 research hours) + 7 hrs in the Summer (research). Most students fulfill the classroom requirements in the first two years, so the third and fourth years of your Ph.D. program would be all research hours.

- Basic student health insurance

For more information and application materials please visit our departmental web site:

http://chem.ou.edu
Oklahoma State University
Department of Chemistry
107 Physical Science
Stillwater, OK 74078

Phone: (405) 744-5920
Fax: (405) 744-6007
http://chem.okstate.edu

Oklahoma State University (OSU) was founded on December 25, 1890, as Oklahoma Agricultural and Mechanical College. The University was renamed Oklahoma State University on July 1, 1957. OSU is located in Stillwater, a north-central Oklahoma community with a population greater than 42,000. Stillwater is approximately one-hour driving distance from the Tulsa and Oklahoma City metropolitan areas.

At OSU, the Department of Chemistry is part of the Arts and Sciences College and is located in two buildings, Physical Sciences I and II. Our undergraduate curriculum includes work in each of four major chemistry subdisciplines—analytical, inorganic, organic, and physical. Students can earn an ACS-certified or a departmental B.S. degree in Chemistry. Over the past five years, 60 students have graduated with the B.S. degree: 40% have begun careers in industry, 15% have attended medical school, and 45% have gone on to graduate study.

Our graduate education program is aimed at the development of a pronounced ability to perform independent creative scientific research. Through carefully selected course work, we provide a firm foundation of skills and knowledge that will enable the student to succeed in both their graduate research project and their subsequent careers. Students usually start research on their thesis topic within the first year after choosing a research advisor and a thesis research topic. Although most students enter immediately into a Ph.D. degree program, a M.S. program is also available.

In both the undergraduate and graduate degree programs, we maintain an excellent faculty to student ratio. For undergraduates, this means personalized attention in the advance courses, access to state of the art instrumentation and the ability to perform cutting edge undergraduate research. For graduate students, the resulting collegial atmosphere is very conducive to faculty/student interaction, collaboration between research groups, and undelayed access to instrumentation.
The OUHSC Graduate College has over 30 MS and PhD degrees in biomedical research and health related research areas. For students interested in chemistry, biochemistry and structural biology OUHSC has MS and PhD degrees in Biochemistry & Molecular Biology and in Pharmaceutical Sciences.

- For additional information on Biochemistry & Molecular Biology see: http://www.oumedicine.com/academictemplate_landing.cfm?id=3842&fr=true.

- For additional on Pharmaceutical Sciences see: http://pharmacy.ouhsc.edu/pharm_sci/.

- For additional information on OUHSC Graduate College and programs see: http://www.ouhsc.edu/graduate/.

The OUHSC Graduate College also provides opportunities for undergraduate students to do research with OUHSC research faculty members. For information on our Summer Undergraduate Research Programs which provide a 9 week summer internship along with housing and a stipend see: http://www.ouhsc.edu/graduate/Summer_Programs.htm.

For information on doing research during the school year for credit, email the OUHSC Graduate College at: gradcollege@ouhsc.edu.
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Our laboratory glassware products include beakers, bottles, burets, cylinders, flasks, pipets, chromatography columns, HPLC (High Performance Liquid Chromatography) mobile phase, distillation, filtration, and extraction systems.

Maria T. DiMaria
Sales and Marketing
Wilmad-LabGlass
maria.dimaria@wilmad-labglass.com

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Lewisville TX 75057  

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Fax: 888-473-9511  
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Mallinckrodt Baker is a unit of Covidien.
Rigaku, the world's leading resource for analytical X-ray instrumentation, components, software and contract services, offers fully integrated crystallography solutions, including microfocus generators; imaging plate and CCD detectors; integrated X-ray optics; and cryo-cooling and humidity control devices. Our bench-top instruments bring affordable, high-performance X-ray fluorescence, diffraction and small molecule crystallography to teaching labs, academia and industry. Our crystal inspection, storage and analysis products integrate every aspect of protein crystallization into an automated and seamless package. Rigaku continuously promotes partnerships, dialog, and innovation within the global scientific and industrial community. Please visit our booth to see how Rigaku can make your valuable research time more productive.

As a leading developer, manufacturer and global supplier of scientific laboratory products for more than 90 years, Corning is the trusted partner of researchers seeking new approaches to increase efficiencies, reduce costs and compress timelines in the drug discovery process. Using our unique expertise in the combined fields of optics, materials science, surfaces, and biology, we provide a full range of innovative solutions that improve productivity and enable breakthrough discoveries.

In addition to being a global leader in consumable glass and plastic laboratory tools for life science research, Corning continues to lead the way with the development and production of the Corning® Epic® System for label-free detection, the HYPERFlask® Cell Culture Vessel for increased cell yields, and novel surfaces such as Ultra-Low Attachment, and the Corning® CellBIND® Surfaces for enhanced assay performance.

We are committed to meeting customers’ unique and changing needs with original solutions for today’s emerging life sciences technologies. Our dedication to quality, technology and innovation continues to enable us to produce the world’s most comprehensive line of drug discovery tools.
Schedule of Events

REGISTRATION
8 AM to 10 AM at Registration Desk near Conference Center Entrance

CONTINENTAL BREAKFAST
8 AM to 9 AM  Ballroom H & I
Sliced Fresh Fruit, Breakfast Breads, Bagels, Fruit Juice, Coffee, Tea

MORNING TECHNICAL SESSIONS

<table>
<thead>
<tr>
<th>Topic</th>
<th>Start Time</th>
<th>End Time</th>
<th>Room</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biofuels – Morning</td>
<td>8:30 AM</td>
<td>11:40 AM</td>
<td>Ballroom J</td>
</tr>
<tr>
<td>Chemical Education/POGIL</td>
<td>8:30 AM</td>
<td>11:40 AM</td>
<td>Sooner B</td>
</tr>
<tr>
<td>Nanotechnology - Biological Applications</td>
<td>8:30 AM</td>
<td>10:00 AM</td>
<td>Ballroom A</td>
</tr>
<tr>
<td>Nuclear Magnetic Resonance</td>
<td>8:30 AM</td>
<td>11:40 AM</td>
<td>Ballroom G</td>
</tr>
<tr>
<td>X-Ray Crystallography</td>
<td>8:30 AM</td>
<td>11:40 AM</td>
<td>Sooner A</td>
</tr>
<tr>
<td>Nanotechnology - Single-Walled Carbon Nanotubes</td>
<td>10:20 AM</td>
<td>11:40 AM</td>
<td>Ballroom A</td>
</tr>
</tbody>
</table>

MORNING COFFEE BREAK
10 AM to 10:20 AM  Ballroom H & I  Soft Drinks, Coffee, Tea

LUNCH BUFFET
12:00 PM to 1:00 PM  Ballroom B & C

2010 OKLAHOMA CHEMIST OF THE YEAR
12:30 PM  Ballroom B & C
Jiten Chatterji, Halliburton Energy Services

BANQUET SPEAKER
12:40 PM  Ballroom B & C
Steve Paris, Oklahoma Center for the Advancement of Science and Technology

AFTERNOON TECHNICAL SESSIONS

Poster Sessions, posters should be displayed all day
9:00 AM  5:00 PM  Ballroom H & I
Poster Authors Present
1:00 PM  2:00 PM

Analysis/Physical Chemistry  Environmental Chemistry  Structural Biology Nexus
Biochemistry  Inorganic Chemistry  Organic Chemistry
Biofuels  Nanotechnology  X-Ray Crystallography
Chemical Education/POGIL  Nuclear Magnetic Resonance

Lecture Sessions

<table>
<thead>
<tr>
<th>Topic</th>
<th>Start Time</th>
<th>End Time</th>
<th>Room</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analytical and Physical Chemistry</td>
<td>2:00 PM</td>
<td>5:10 PM</td>
<td>Ballroom B</td>
</tr>
<tr>
<td>Biochemistry</td>
<td>2:00 PM</td>
<td>3:30 PM</td>
<td>Ballroom G</td>
</tr>
<tr>
<td>Biofuels - Afternoon</td>
<td>2:00 PM</td>
<td>5:10 PM</td>
<td>Ballroom J</td>
</tr>
<tr>
<td>Nanotechnology - Tubes and Rods</td>
<td>2:00 PM</td>
<td>3:30 PM</td>
<td>Ballroom A</td>
</tr>
<tr>
<td>Organic Chemistry</td>
<td>2:00 PM</td>
<td>3:30 PM</td>
<td>Ballroom C</td>
</tr>
<tr>
<td>Environmental Chemistry</td>
<td>3:50 PM</td>
<td>6:00 PM</td>
<td>Ballroom G</td>
</tr>
<tr>
<td>Inorganic Chemistry</td>
<td>3:50 PM</td>
<td>5:30 PM</td>
<td>Sooner A</td>
</tr>
<tr>
<td>Nanotechnology - Materials</td>
<td>3:50 PM</td>
<td>5:30 PM</td>
<td>Ballroom A</td>
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<tr>
<td>Pharmacology/Natural Products</td>
<td>3:50 PM</td>
<td>6:00 PM</td>
<td>Ballroom C</td>
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</tbody>
</table>

AFTERNOON COFFEE BREAK
3:30 PM to 3:50 PM  Ballroom H & I
“Chef’s Sweet of the Day” and “PM Protein Break” plus Soft Drinks, Coffee, Tea.

[ 17 ]
2010 Oklahoma ACS Section Officers & Standing Committee Chairs

Nicholas F. Materer  Chair
Amanda J. Nichols  Chair Elect
Lloyd A. Bumm  Immediate Past Chair
Lloyd A. Bumm  Secretary
Kenneth H. Brown  Treasurer
Allen Apblett  Councilor + Nominations Committee
Donna J. Nelson  Alternate Councilor
Charles V. Rice  Awards Committee
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Valerie Ferguson  National Chemistry Week Committee
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For more information, visit the website of the Oklahoma Section of the American Chemical Society.
http://oklahoma.sites.acs.org/

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—The Oklahoma Section of the ACS Executive Committee
Lecture Sessions at the
55th Annual Pentasectional Meeting of the
American Chemical Society

Conference Chairs: Charles Rice (Chemistry & Biochemistry, University of Oklahoma)
Lloyd Bumm (Physics, University of Oklahoma)

Saturday, April 10, 8:00 AM to 6:00 PM

8:30 T1 Exhibitors - Ballrooms H and I
Charles Rice, Chemistry and Biochemistry, University of Oklahoma

12:30 T2 Oklahoma Chemist of the Year - Ballrooms B and C
Jiten Chatterji, Halliburton Energy Services

12:40 T3 Banquet Speaker - Ballrooms B and C
Steve Paris, public information officer, Oklahoma Center for the Advancement of Science and Technology (OCAST), will give a presentation on the Oklahoma Applied Research Support program, known as OARS.

2:00 T4 Future Meeting Planning Session - Sooner A
Nicholas Materer, Department of Chemistry, Oklahoma State University

Saturday, April 10, 8:30 AM. S2: Biofuels - Morning

Presider: Richard Mallinson (Chemical, Biological, and Materials Engineering, OU)
Room: Ballroom J

8:30 T5 Experimental Investigation of Flame Characteristics of Canola Methyl Ester and Jet-A Blends in a Porous Media Burner
Balasaheb Dahifale, Aerospace and Mechanical Engineering, University of Oklahoma

8:50 T6 Measurement of Drag Coefficients of Biofuel Droplets in Free Fall
Diana Martinez, Aerospace and Mechanical Engineering, University of Oklahoma

9:10 T7 Soot Particle Analysis in Air-Flames of Canola Methyl Ester Biofuel and Diesel Fuel
Wilson Merchán-Merchán, Aerospace and Mechanical Engineering, The University of Oklahoma

9:30 T8 Analysis of the Relative Fatty Acid Contents of Base and Acid Catalyzed Biodiesel
Petar Petrov, Chemistry, University of Central Oklahoma

10:00 BREAK
10:20 T9 Condensation Reactions of Propanal over Ceria-Zirconia Mixed Oxide Catalysts
Anirudhan Gangadharan, School of Chemical, Biological and Materials Engineering, University of Oklahoma

10:40 T10 Catalytic Upgrading of Switchgrass Pyrolysis Bio-oil Vapors over Ce$_{0.5}$Zr$_{0.5}$O$_2$ Mixed Oxide Catalyst
Jonathan Peters, School of Chemical, Biological, and Materials Engineering, University of Oklahoma

11:00 T11 Selective Deoxygenation of Furfuraldehyde on Bimetallic Catalysts
Surapas Sitthisa, School of Chemical, Biological and Materials Engineering, The University of Oklahoma

11:20 T12 Reactions of 2-Methylpentanal on Bimetallic Pd-Cu Catalysts
Trung Pham, Chemical Engineering, University of Oklahoma

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Saturday, April 10, 8:30 AM. S3: Chemical Education/POGIL

Presider: Michael Abraham (Chemistry & Biochemistry, The University of Oklahoma)
Room: Sooner B

8:30 T13 Adapting a Methodology for Documenting Collective Growth to an Undergraduate Physical Chemistry Class
Renee Cole, Biochemistry, Chemistry & Physics, University of Central Missouri

8:50 T14 A New Approach to General Chemistry: Switching from Topics to Questions
Vicente Talanquer, Chemistry and Biochemistry, University of Arizona

9:10 T15 Teaching Chemistry with Visualization
Vickie Williamson, Chemistry, Texas A & M University

9:30 T16 Inquiry in Large Class Settings: Before, During, and After Class Activities
Michael Abraham, Chemistry & Biochemistry, The University of Oklahoma

9:50 Discussion

10:00 BREAK

10:20 T17 POGIL in a Large Enrollment Organic Chemistry I Course
Mark Morvant, Chemistry & Biochemistry, University of Oklahoma

10:40 T18 Getting from "Wow!" to "Aha!: Using POGIL to Spur Learning From Demonstrations
Stephen Prilliman, Chemistry, Oklahoma City University

11:00 T19 Math as a Second Language: A New Model for Math Literacy in the Science Classroom
Benjamin Sandler, Biochemistry, Oklahoma State University

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11:20 T20 Use of a Spreadsheet to Calculate the Net Charge of Peptides and Proteins as a Function of pH: an Alternative to Using "Canned" Programs to Estimate the Isoelectric Point (pI) of These Important Biomolecules
Paul Sims, Chemistry & Biochemistry, The University of Oklahoma

11:40 Discussion

Saturday, April 10, 8:30 AM. S4: Nanotechnology - Biological Applications
Presider: Donna Nelson (Chemistry & Biochemistry, The University of Oklahoma)
Room: Ballroom A

8:30 T21 Targeted Nano-Biological Probes for Tumor Markers Visualized by Molecular Magnetic Resonance Imaging (mMRI)
Rheal Towner, Advanced Magnetic Resonance Center, Oklahoma Medical Research Foundation

8:50 T22 Novel Magnetic Nanoparticles for Gene Delivery in Mesenchymal Stem Cells
Ananta Ayyagari, Department of Chemistry and Biochemistry, University of Oklahoma

9:10 T23 Using Fluorescent Nanoparticles for Transfection of Plant Cells
Jeanmarie Verchet-Lubicz, Entomology and Plant Pathology, Oklahoma State University

9:30 T24 Virus Enabled Photosensitizer for Photodynamic Therapy in Breast Cancer Cells
Naveen Gandra, Chemistry and Biochemistry, University of Oklahoma

Saturday, April 10, 8:30 AM. S5: Nuclear Magnetic Resonance
Presider: Susan Schroeder (Chemistry and Biochemistry, University of Oklahoma)
Room: Ballroom G

8:30 T25 Tying up the Ends: Recognition of ssDNA at Telomeres
Deborah Wuttke, Chemistry and Biochemistry, University of Colorado

9:20 T26 NMR Structure of phi29 Prohead RNA E-loop Hairpin
Steven Harris, Chemistry and Biochemistry, The University of Oklahoma

9:40 T27 NMR Studies of human MID1, a Novel E3 Ligase Targeting Protein Phosphatase 2A
Michael Massiah, Biochemistry & Molecular Biology, Oklahoma State University

10:00 T28 Novel Insights of Protein Aggregation by NMR
Valentin Sluch, Biochemistry and Molecular Biology, Oklahoma State University

10:10 BREAK

10:20 T29 Protein Structure Determination by Magic-Angle Spinning Solid-State NMR
Donghua Zhou, Physics, Oklahoma State University
10:40 T30 An NMR View Polymer-Plasticizer Interactions
Frank Blum, Chemistry, Oklahoma State University

11:00 T31 Cadmium Chelation by Bacterial Teichoic Acid from Solid-State NMR Spectroscopy
Jeffrey Halye, Chemistry and Biochemistry, The University of Oklahoma

11:20 T32 Multi-Receiver NMR
Yasvir Tesiram, Advanced Magnetic Resonance Center, Oklahoma Medical Research Foundation

Saturday, April 10, 8:30 AM. S6: X-Ray Crystallography
Presider: Leonard Thomas (Chemistry & Biochemistry, The University of Oklahoma)
Room: Sooner A

8:30 T33 The Distal Pocket Histidine Residue in Horse Heart Myoglobin Directs the O-Binding Mode of Nitrite to the Heme Iron
Jun Yi, Chemistry and Biochemistry, The University of Oklahoma

8:50 T34 Understanding the Architecture and Assembly of Large Double-Stranded DNA Icosahedral Viruses
Stacy Benson, Chemistry, Oklahoma State University

9:10 T35 Crystal Structure of an Eight-Base Pair Fragment from a U-tail Helix Domain from RNA Editing Complexes in Trypanosoma brucei
Blaine Mooers, Biochemistry and Molecular Biology, University of Oklahoma Health Sciences Center

9:30 T36 Structural Biology Study of Biosynthesis of Plant Natural Products
Hui Shao, Plant Biology Division, The Samuel Roberts Noble Foundation

10:00 BREAK

10:20 T37 X-Ray Crystal Structure of Acetyl Esterase from Escherichia coli
Mamiko Nishida, Chemistry, Oklahoma State University

10:40 T38 Rejuvenating a Classic Antimicrobial Target for Today’s Anti-Bacterial Needs
Christina Bourne, Veterinary Pathobiology, Oklahoma State University

11:00 T39 IL18 & IL18BP in Autoimmune and Infectious Diseases
Junpeng Deng, Biochemistry and Molecular Biology, Oklahoma State University
Saturday, April 10, 10:20 AM. S4: Nanotechnology - Single-Walled Carbon Nanotubes

Presider: Christopher Brammer (Chemistry & Biochemistry, The University of Oklahoma)
Room: Ballroom A

10:20 T40 Effects of NaHCO₃ Washing and Change in Reagent Order upon the Reaction of Single-Walled Carbon Nanotubes with Thionyl Chloride and PMMA
Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma

10:40 T41 Horizontally Aligned Single Walled Carbon Nanotubes (SWNTs): Effect of H₂O on Defect Density and Film Uniformity
Wesley Tennyson, School of Chemical, Biological & Materials Engineering, The University of Oklahoma

11:00 T42 Controlled Functionalization of Single-Walled Carbon Nanotubes with TEMPO-ended Polystyrene
Abhijit Paul, Chemistry, Oklahoma State University

11:20 T43 Synthesis of Functionally Graded Nanocoatings Using Initiated Chemical Vapor Deposition (iCVD)
Yumin Ye, Biosystems Engineering, Oklahoma State University

Saturday, April 10, 2:00 PM. S7: Analytical and Physical Chemistry

Presider: Ivan Yip (Chemistry & Biochemistry, The University of Oklahoma)
Room: Ballroom B

2:00 T44 Electron Transfer Assisted Intersystem Crossing in Cyanoaromatics
Paritosh Das, Physical Sciences, Cameron University

2:20 T45 Controlling the Amount of Dye Loaded on a Nanoparticle Surface
Ronald Halterman, Chemistry and Biochemistry, The University of Oklahoma

2:40 T46 Quantification of Total ω-6, Total ω-3 and ω-6/ω-3 Ratio and Validation of Purdie Assay Using GC-MS
Mary Kimani, Chemistry, Oklahoma State University

3:00 T47 Pd Nanoclusters on Pristine and Functionalized Single-Wall Carbon Nanotube: DFT and Experimental Studies
Teerawit Prasomsri, Chemical Engineering, The University of Oklahoma

3:20 Discussion

3:30 BREAK

3:50 T48 Silver-Alkenethiol Interaction Monitored from Plasmon Resonance
Rama Krishna Ede, Department of Mechanical and Aerospace Engineering, Oklahoma State University
4:10  T49  Carbon Dioxide Generated In Situ by Carbamate for EOR Application
Tzu-Ping Hsu, Petroleum Engineering, The University of Oklahoma

4:30  T50  Micelle Simulations with GB Implicit-Solvent Models: Parameterization and Application to pKa Predictions of Surfactants in Micelles
Yuhang Wang, Chemistry and Biochemistry, The University of Oklahoma

4:50  T51  Vibrational Spectroscopic and X-Ray Crystallographic Study of Secondary Amine/Phosphoric Acid Systems
Dharshani Bopege, Physics & Astronomy, The University of Oklahoma

Saturday, April 10, 2:00 PM. S8: Biochemistry
Presider: Paul Sims (Chemistry & Biochemistry, The University of Oklahoma)
Room: Ballroom G

2:00 T52  The Neuraminidase Activity of Human Parainfluenza Viruses 1, 2, and 3
Mary Tappert, Biochemistry and Molecular Biology, University of Oklahoma Health Sciences Center

2:20 T53  Functional Role of Active Site Residues, Glu78, Glu122, H96 and Lys99 of Saccharopine dehydrogenase from Saccharomyces cerevisiae
Devi Ekanayake, Department of Chemistry and Biochemistry, The University of Oklahoma

2:40 T54  Mechanism of Homocitrate Synthase
Vidya Kumar, Chemistry and Biochemistry, The University of Oklahoma

3:00 T55  Mutational Analysis of Bacterial Condensin MukBEF
Weifeng She, Chemistry and Biochemistry, The University of Oklahoma

3:20 T56  Reconstitution of Macrolide Pump MacAB-TolC into Lipid Nanodiscs
Shuo Lu, Chemistry and Biochemistry, The University of Oklahoma

Saturday, April 10, 2:00 PM. S2: Biofuels - Afternoon
Presider: Richard Mallinson (Chemical, Biological, and Materials Engineering, OU)
Room: Ballroom J

2:00 T57  Conversion of Methyl Esters on Supported Pt Catalysts
Phuong Do, Chemical Engineering, The University of Oklahoma

2:20 T58  Conversion of Lauric Oils on Platinum Supported Catalysts
Kyle Elam, Chemical, Biological, and Materials Engineering, The University of Oklahoma
Vanadyl meso-Tetraphenylporphyrin Catalyzed Pinacol Coupling Reactions in Water
Ronald Halterman, Chemistry and Biochemistry, The University of Oklahoma

Nanohybrid Particles that Catalyze Biofuel Upgrade Reactions at the Interface Of Water/Oil Emulsions
Jimmy Faria, Chemical, Biological and Materials Engineering, University of Oklahoma

BREAK

Model Compound Study of Phenolic Compounds Conversion over Acidic Zeolites During Bio-Oil Upgrading
Xinli Zhu, School Of Chemical Biological And Materials Engineering, The University of Oklahoma

Saturday, April 10, 2:00 PM. S4: Nanotechnology - Tubes and Rods
Presider: Allen Apblett (Chemistry, Oklahoma State University)
Room: Ballroom A

Synthesis of SWNT-Silica-Polystyrene Composites by Pickering Miniemulsion Polymerization
Min Shen, Chemical Engineering, The University of Oklahoma

Interfacially Active SWNT/Silica Nanohybrid Used in Enhanced Oil Recovery
Luis Villamizar, Petroleum Engineering, The University of Oklahoma

Counter-Flow Diffusion Flame Synthesis of Polygonal and Ribbons-Like Tungsten Oxide Nanostructures
Wilson Merchan-Merchan, Aerospace and Mechanical Engineering, The University of Oklahoma

Novel Nanovectors for Targeted SKBR-3 Breast Cancer Cell Imaging and Destruction
Gopal Abbineni, Chemistry & Biochemistry, The University of Oklahoma
Saturday, April 10, 2:00 PM. S9: Organic Chemistry  
**Presider:** Donna Nelson (Chemistry & Biochemistry, The University of Oklahoma)  
**Room:** Ballroom C

2:00 T66 **Hollywood Chemistry**  
Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma

2:20 T67 **Effects of Ligand Structure and Donor Type on Catalytic Activities of Electrophilic (Chelate)Palladium(2+) Complexes**  
LeGrande Slaughter, Chemistry, Oklahoma State University

2:40 T68 **Ligand-Accelerated Intramolecular Amination**  
Dipti Barman, Chemistry and Biochemistry, The University Of Oklahoma

3:00 T69 **Synthesis of Metabolites of the Heteroarotinoid Drug SHetA2**  
Baskar Nammalwar, Department of Chemistry, Oklahoma State University

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Saturday, April 10, 3:50 PM. S10: Environmental Chemistry  
**Presider:** Mark Nanny (School of Civil Engineering & Environmental Science, The University of Oklahoma)  
**Room:** Ballroom G

3:50 T70 **Using Solid-State Deuterium NMR to Characterize the Association of Benzene With Humic and Fulvic Acids**  
Mark Nanny, School of Civil Engineering & Environmental Science, The University of Oklahoma

4:10 T71 **Individualization of Gasolines by GCIRMS Fingerprinting**  
Tomasz Kuder, Geology, The University of Oklahoma

4:30 T72 **Characterization of Naphthenic Acids in Petroleum Process Waste Water**  
Mark Nanny, School of Civil Engineering & Environmental Science, The University of Oklahoma

5:00 T73 **Enhancing Microbial Methanogenesis of Coal by Ozonolysis**  
Mark Nanny, School of Civil Engineering & Environmental Science, The University of Oklahoma

5:20 T74 **Environmental, Synthetic, and Materials Applications of Tungsten Trioxide**  
Hamed Albusaidi, Chemistry, Oklahoma State University

5:40 T75 **Green Chemistry Laboratory: Molybdate Processing of Copper Ore**  
Kevin Barber, Chemistry, Oklahoma State University
Saturday, April 10, 3:50 PM. S11: Inorganic Chemistry
Presider: Doug Powell (Department of Chemistry & Biochemistry, University of Oklahoma)
Room: Sooner A

3:50 T76 Synergism in the Flame Retardancy of Guanyl Urea Phosphate and Boric Acid Mixture on Polyurethane Foam.
Bhawani Regmi, Chemistry, Oklahoma State University

4:10 T77 Synthetic and Mechanistic Studies of Migratory Insertion of CO into Cationic Methylpalladium Complexes Containing bis N-Heterocyclic Carbene (bis-NHC) Ligands
Sri Subramaniam, Chemistry, Oklahoma State University

4:30 T78 Crystallographic Analysis of Organometallic Structures with Extended Metallophilic and Pi-Pi Interactions
LeGrande Slaughter, Chemistry, Oklahoma State University

4:50 T79 Light-Induced Transformation of Nanostructured V₃O₇·H₂O to V₂O₅
C. Ozge Topal, Department of Mechanical and Aerospace Engineering, Oklahoma State University

5:10 T80 Silica Gel Supported Titanium Catalyzed Conversion of Benzyl Phenyl Ketone and Diphenylacetylene to Benzaldehyde.
Robert Cannon, Chemistry, Oklahoma State University

Saturday, April 10, 3:50 PM. S4: Nanotechnology - Materials
Presider: Donna Nelson (Chemistry & Biochemistry, The University of Oklahoma)
Room: Ballroom A

3:50 T81 Strength Improvement via Coating of a Cylindrical Hole by Layer-by-Layer Assembled Polymer Particles
Brian Grady, Chemical, Biological and Materials Engineering, The University of Oklahoma

4:10 T82 Nanowire-Nanoparticle Conjugate Photolytic Fuel Generators
Kaan Kalkan, Mechanical and Aerospace Engineering, Oklahoma State University

4:30 T83 Silica Incorporated Titania Semicoducting Nanoparticles: Transmission IR Studies Towards Photocatalysis
Dilip Paul, Chemistry, Pittsburg State University

4:50 T84 Electrochemical Characterization of SnO₂ Nanobasket Electrodes with Capacities Exceeding Theoretical Values
Matthew Smith, Department of Chemistry and Biochemistry, University of Tulsa

5:10 T85 Nanotechnology for Neutralization of Explosives in the Field and the Laboratory
Allen Apblett, Chemistry, Oklahoma State University
Saturday, April 10, 3:50 PM. S12: Pharmacology/Natural Products

**Presider:** Robert Cichewicz (Chemistry & Biochemistry, The University of Oklahoma)

**Room:** Ballroom C

3:50 T86  **Biosynthesis of Glycosides - Glycosyltransferase Structures and Engineering**  
Xiaoqiang Wang, Plant Biology Division, The Noble Foundation

4:10 T87  **Metabolomics and Integrated Functional Genomics Reveal Novel Information Related to Medicago Secondary Metabolism**  
Zhentian Lei, Plant Biology Division, The Noble Foundation

4:30 T88  **Chemical Epigenetic Manipulation of Secondary Metabolite Production by a Penicillium citreonigrum Isolate Obtained from the Atlantic Forest**  
Xiaoru Wang, Chemistry and Biochemistry, The University of Oklahoma

4:50 T89  **Naturally-Occurring Triterpenoids as Potential Anticancer Agents: Prevention and Treatment of Colorectal Cancer**  
Chinthalapally Rao, Medicine, University of Oklahoma Health Sciences Center

5:10 T90  **Anti-Cancer Action of Frankincense Oil from Boswellia species**  
Hsueh-Kung Lin, Urology, University of Oklahoma Health Sciences Center

5:30 T91  **Dried Plum Extract Reverses Osteopenia by Altering Osteoblast and Osteoclast Differentiation and Activity**  
Brenda Smith, Department of Nutritional Sciences, Oklahoma State University
Poster Sessions at the 55th Annual Pentasectional Meeting of the American Chemical Society

Conference Chairs: Charles Rice (Chemistry and Biochemistry, University of Oklahoma)
Lloyd Bumm (Physics, University of Oklahoma)

Saturday, April 10, 1:00 PM in Ballrooms H and I

Posters should be ready for display by 10 AM and taken down after 4 PM

Analytical/Physical - Poster Session

Room: Ballrooms H and I

P1 Adsorption and Reaction of Propene on Different Cationic Forms of Y Zeolite: Prediction of Polymerization Activity from IR Molar Absorption Coefficients.
Kassie (ThuHuong) Ngo, Chemical, Biological and Materials Engineering, The University of Oklahoma

P2 Analysis and Quantitation of Phthalate Plasticizers in Surface Waters Using SPME/GC-MS
Basil Mathews, Chemistry, University of Central Oklahoma

P3 Catalytic Isomerization of N-Butane on H-Mordenite: Influence of Hydrogen Partial Pressure
Matt Wulfers, Chemical, Biological and Materials Engineering, University of Oklahoma

P4 Charge-Transfer Mediated Photchemistry of Small-Ring Systems.
Paritosh Das, Physical Sciences, Cameron University

P5 Correlation of Hydrogen Bonding Species in N,N’-DMEDA and N,N’-DMPDA and Their Complexes with Lithium Trifluoromethanesulfonate with Infrared and Raman Vibrational Band
Rachel Mason, Chemistry & Biochemistry, The University of Oklahoma

P6 Developing Surfactant Formulation for Oil-Wet Carbonate Formations
Oluwafemi Afelumo, Petroleum Engineering, The University of Oklahoma

P7 Differential Pulse Anodic Stripping Voltammetry (DPASV) for the Detection of Barium from Oil Well Water
Crystal Mars, Chemistry and Physics, Southwestern Oklahoma State University

P8 Environmental and Galvanic Corrosion Rates for Iron and Zinc Wires
Ahmad Razzaghi, Chemistry, Oklahoma State University

Srinivas Hanumansetty, Chemical, Biological and Materials Engineering, The University of Oklahoma
Biochemistry - Poster Session
Room: Ballrooms H and I

P14  Altered Sensitivity to MDMA in Mice Made Tolerant to the Hallucinogen DOI
Jacob Hostetler, Oral Roberts University

P15  Cloning And Characterization Of Yeast Aminotransferase
Lilian Chooback, Chemistry, University Of Central Oklahoma

P16  Cloning Of CaSSK1, A Gene That Expresses An Oxidative Stress Protein From Candida albicans
Hui Tan, Physical Sciences Department, Cameron University

P17  Early Events During the Reaction of Hypochlorous Acid with Escherichia coli Cells
Bockim Lee, Chemistry and Biochemistry, The Oklahoma University

P18  Experimental Restraints Reduce Folding Space and Enable Computation of a Complete Set of Possible Folding Solutions for a Viral RNA
Jonathan Stone, Chemistry and Biochemistry, The University of Oklahoma

P19  Experimental Restraints Reduce Folding Space and Enable Computation of a Complete Set of Possible Folding Solutions for a Viral RNA
Montana Rowe, Chemistry and Biochemistry, The University of Oklahoma

P20  Influence of Salivary Defensive Peroxidases on Streptococcal Antagonism in Oral Biofilms
Michael Ashby, Chemistry and Biochemistry, The University of Oklahoma

P21  Is Cyanogenesis a Virulence Factor of Pseudomonas aeruginosa that Inactivates Human Defensive Peroxidases and their Antimicrobial Hypohalites?
Michael Ashby, Chemistry and Biochemistry, The University of Oklahoma
[ POSTER PROGRAM ]

P22  Mechanism of the Stimulation of MacB ATPase by the Periplasmic Membrane Fusion Protein (MFP) MacA
Sita Devi Modali, Chemistry and Biochemistry, The University of Oklahoma

P23  Midline-1 Has 3 RING Fold Domains which all have E3 Ligase Activity
Xiaofeng Han, Biochemistry And Molecular Biology, Oklahoma State University

P24  Prohead RNA Self-Assembly
Xiaobo Gu, Chemistry and Biochemistry, The University of Oklahoma

Koree Clanton Arrowood, Chemistry and Biochemistry, The University of Oklahoma

Biofuels - Poster Session
Room: Ballrooms H and I

P26  An Efficient Catalytic Deoxydehydration Reaction for the Conversion of Biomass-Derived Glycols to Alkenes
Irshad Ahmad, Chemistry and Biochemistry, The University of Oklahoma

P27  Anaerobic Biodegradation of Biodiesel and Corrosion
Deniz F. Aktas, Botany and Microbiology, The Univeristy of Oklahoma

P28  Catalytic Conversion of Diols to Alkene via Epoxide
A.K. Fazlur Rahman, Chemistry, Oklahoma School of Science and Mathematics

P29  Methyltrioxorhenium Catalyzed Deoxydehydration of Glycols and Epoxides to Alkenes utilizing Sodium Sulfite as a Reductant
Garry Chapman Jr., Chemistry and Biochemistry, The University of Oklahoma

P30  New Biofuel Cell Anode Materials Based on Linear Poly(Ethlenimine) and Ferrocene
Matt Meredith, Chemistry and Biochemistry, The University of Oklahoma

Chemical Education/POGIL - Posters Session
Room: Ballrooms H and I

P31  Metal-Oxalate Complex Salts: Teaching an Old Lab New Tricks
Stephen Prilliman, Chemistry, Oklahoma City University

P32  Preparation and Infrared Spectroelectrochemistry of Iron Dinitrosyl Compounds: Towards an Undergraduate Research Experience
Myron Jones, Chemistry and Biochemistry, The University of Oklahoma

[ 31 ]
P33 Teaching Column Chromatography: Open-Ended Approach for Understanding Lab Techniques
Keegan Long-Wheeler, Chemistry and Biochemistry, The University of Oklahoma

P34 The Spectroscopy of Stars and Applications for Students
Stephen Prilliman, Chemistry, Oklahoma City University

Environmental Chemistry - Poster Session
Room: Ballrooms H and I

P35 A Model of Anaerobic Oxidation of Methane via The Fumarate Addition Mechanism Using DFT Calculations
Keisha Beasley, CEES, The University of Oklahoma

P36 Comparison of Methyl Glucamine and Glycoside Surfactant Headgroup Synergism with Alkyl Carboxylic Acid Salts
Louis Jackson, Engineering, The University of Oklahoma

Inorganic Chemistry - Poster Session
Room: Ballrooms H and I

P37 Bio-Coordination Chemistry: Transition Metal CXCR4 Antagonists
Tim Hubin, Chemistry, Southwestern Oklahoma State University

P38 Hydroxamate Iron Porphyrinates As New Synthetic Model For The Active Site Of Catalase
Adam Warhausen, Chemistry and Biochemistry, The University of Oklahoma

P39 Improved Synthesis of Sodium Molybdenum Bronze
Cory Perkins, Chemistry, Oklahoma State University

P40 Organoruthenium Porphyrins With O-Bound Ligands Trans To Nitric Oxide
Dennis Awasabisah, Chemistry and Biochemistry, The University of Oklahoma

P41 Structural Investigations into the Heme Nitrosamine Interaction
Nan Xu, Chemistry and Biochemistry, The University of Oklahoma

P42 Synthesis and Biological Studies of Nicotinic Acid and Thionicotinic Acid Metal Complexes
A.K. Fazlur Rahman, Chemistry, Oklahoma School of Science and Mathematics
Nanotechnology - Poster Session
Room: Ballrooms H and I

P43  Capillary Electrophoresis Separations Of Nanoparticles
    Thushara Athauda, Chemistry and Biochemistry, University Of Tulsa

P44  Characterization Of Multiwalled Carbon Nanotube Polymer Composites
    Robert Headrick, Research and Development, SouthWest Nano Technologies

P45  Controlled Growth And Differentiation Of Mesenchymal Stem Cells On
    Bacteriophage Films
    Haibao Zhu, Chemistry and Biochemistry, The University of Oklahoma

P46  Development And Characterization Of Fast-Acting Microspheres For
    Thrombolytic Therapy
    Hoai Nguyen, Chemical, Biological and Materials Engineering, University of
    Oklahoma

P47  Effect of Single-Walled Carbon Nanotube Association upon Representative
    Organonitrogen Compounds
    Donna Nelson, Chemistry and Biochemistry, The University of Oklahoma

P48  Effects of Sodium Bicarbonate Treatment on the Structure of Single Walled
    Carbon Nanotube Brands Studied by Raman and Ultraviolet-Visible Spectroscopy
    Donna Nelson, Chemistry and Biochemistry, The University of Oklahoma

P49  Emulsion Systems Stabilized And Catalyzed By Janus-Silica-Nanoparticles-
    Supported Catalysts
    Maria Ruiz, Chemical, Biological & Materials Engineering, University of Oklahoma

P50  Evaluation Of Liposome Encapsulated Hemoglobin In Hemorrhagic Shock By
    Mr Spectroscopy
    Hrushikesh Agashe, Pharmaceutical Sciences, College of Pharmacy

P51  Florescence and Raman Spectroscopy of Carbon Nanotubes
    Chase Brown, Lab, Southwest Nanotechnologies

P52  Formation Of Hydrophobic Thin Film on Cotton by Admicellar Polymerization
    Pratik Kothary, Chemical Engineering, The University of Oklahoma

P53  Improved Electrical Conductivities Of SWNT/Silica Hybrid And UHMWPE
    Composites Prepared By Sintering Method
    Cristina Caamano, Chemical, Biological and Materials Engineering, The University
    of Oklahoma

P54  Influence of the Silica Catalyst Support on the Chirality Distribution of Single
    Wall Carbon Nanotubes
    Tyler Ledlow, The University of Oklahoma
P55  Known and Predictable MWNT Structure by Adjusting Metal-Support Interactions in Active Catalysts
Veronica Irurzun, Chemical, Biological & Materials Engineering, The University of Oklahoma

P56  Mixing in Dyeing Equipment, Process Scaling Up for Making Cotton Fabric Water Repellent
Srinivas Hanumansetty, Chemical, Biological and Materials Engineering, The University of Oklahoma

P57  Nanotechnology Utilizing Nanometric Molybdenum And Hydrogen Bronze Reagents For The Neutralization Of Explosives.
Derek Bussan, Chemistry, Oklahoma State University

P58  Percolation Behavior of Multi-Walled Carbon Nanotubes / High-Density Polyethylene Composites
Frank Yepez Castillo, Chemical, Biological and Materials Engineering, The University of Oklahoma

P59  Photocatalytic activity towards Acetaldehyde over Doped Semiconducting Nanoparticles
Dilip Paul, Chemistry, Pittsburg State University

P60  Preparation and Comparison of Hydrophobic Cotton Fabric obtained by Direct Fluorination and Admicellar Polymerization of Fluoromonomers
Pratik Kothary, Chemical Engineering, The University of Oklahoma

P61  Silica encapsulation of Luminescent CdSe/ZnS Nanoparticles
Naga Koduri, Chemistry and Biochemistry, University of Tulsa

NMR - Poster Session
Room: Ballrooms H and I

P62  Glass Transitions, Segmental Dynamics, and Friction Coefficients for Individual Polymers in Multicomponent Polymer Systems by Chain-Level Experiments
Lance Gill, Chemistry, Oklahoma State University

P63  NMR structural Studies of the C Terminal Domain of Alpha4, a PP2A Regulator
Haijuan Du, Biochemistry and Molecular Biology, Oklahoma State University

P64  Solid-State NMR Investigation of Lipid Storage Droplet Protein-1
Liying Wang, Physics, Oklahoma State University
Structural Biology Nexus - Posters Session
Room: Ballrooms H and I

P65  In situ Generation of Ferrous Myoglobin Nitrite Using Synchrotron Induced X-Ray Photoreduction
George Richter-Addo, Chemistry and Biochemistry, The University of Oklahoma

P66  Nitrosoalkane Adducts of Human Hemoglobin
Guan Ye, Chemistry and Biochemistry, University of Oklahoma

P67  Probing The Strand Orientation And Registry Alignment In The Propagation Of Amyloid Fibrils
Jason Wallace, Chemistry and Biochemistry, The University of Oklahoma

Organic Chemistry - Poster Session
Room: Ballrooms H and I

P68  (±)-1-Alkyl-2-aryl-6-nitro-4-oxo-1,2,3,4-tetrahydroquinoline-3-carboxylate Esters by a Tandem Imine Addition-SNAr Reaction
James Schammerhorn, Chemistry, Oklahoma State University

P69  Consistency Among Influences upon Alkene Selenenylation in Chiral Induction, Stereochemistry, Relative Reactivities, and Their Comparisons with Sulfur Analogs
Donna Nelson, Chemistry and Biochemistry, The University of Oklahoma

P70  Development of Chiral Zinc Complexes for Esterolytic Kinetic Resolutions: Exploration of Dynamic Combinatorial Catalysis
Ramu Kannappan, Chemistry and Biochemistry, University of Oklahoma

P71  Ethyl 4-Oxo-1,4-dihydroquinoline-3-carboxylates by a Tandem Addition-Elimination-SNAr Reaction
Eric Lee, Chemistry, Oklahoma State University

P72  Novel Imageable 3,5-Bis(2-Fluorobenzylidene)-4-Piperidone For PET Imaging
Pallavi Lagisetty, Pharmaceutical Sciences, University of Oklahoma Health Sciences Center

P73  One Pot Synthesis of Aryl- and Alkyl-substituted Dihydroquinazolinone Rings By a Dissolving Metal Reduction Process
Baskar Nammalwar, Chemistry, Oklahoma State University

P74  Phenylamine Functionalization of Single-Wall Carbon Nanotubes
David Martyn, Chemistry and Physics, Southwestern Oklahoma State University

P75  Synthesis of Ferrocene-Modified Polypyrrole for Application as a Molecular Wire in REDOX Polymer Biosensors
David Hickey, Chemistry and Biochemistry, The University of Oklahoma
P76  **Synthesis of Resveratrol**  
Dustin Sprouse, Biology and Chemistry, Oral Roberts University

P77  **Toward Consistent Terminology for Cyclohexane Conformers in Introductory Organic Chemistry**  
Donna Nelson, Chemistry and Biochemistry, The University of Oklahoma

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**X-Ray Crystallography - Poster Session**  
**Room:** Ballrooms H and I

P78  **Crystallographic Study of a Novel Cinnamyl Alcohol Dehydrogenase**  
Haiyun Pan, Plant Biology Division, The Samuel Roberts Noble Foundation

P79  **Preliminary Crystallographic Study of Galactosyltransferase GalT1**  
Qing Chang, Plant Biology Division, The Samuel Roberts Noble Foundation

P80  **Structure Function Studies Of Vaccinia Virus Host-Range Protein K1 Reveal A Novel Functional Surface For Ankyrin-Repeat Proteins**  
Yongchao Li, Biochemistry and Molecular Biology, Oklahoma State University
LECTURE ABSTRACTS

8:30 AM - 11:40 AM Ballroom J
S2: Biofuels - Morning
Chair and Presider: Richard Mallinson
(Chemical, Biological and Materials Engineering, OU)

8:30 T5 Experimental Investigation of Flame Characteristics of Canola Methyl Ester and Jet A Blends in a Porous Media Burner

8:50 T6 Measurement of Drag Coefficients of Biofuel Droplets In Free Fall

9:10 T7 Soot Particle Analysis in Air-Flames of Canola Methyl Ester Biofuel and Diesel Fuel

9:30 T8 Analysis of the Relative Fatty Acid Contents of Base and Acid Catalyzed Biodiesel

10:00 BREAK

10:20 T9 Condensation Reactions of Propanal over Ceria-Zirconia Mixed Oxide Catalysts

10:40 T10 Catalytic Upgrading of Switchgrass Pyrolysis Bio-Oil Vapors Over Ce0.5Zr0.5O2 Mixed Oxide Catalyst

11:00 T11 Selective Deoxygenation of Furfuraldehyde on Bimetallic Catalysts

11:20 T12 Reactions of 2-Methylpentanal on Bimetallic Pd-Cu Catalysts

T5: Experimental Investigation of Flame Characteristics of Canola Methyl Ester and Jet A Blends in a Porous Media Burner
Presenter: Balasaheb Dahifale, Aerospace and Mechanical Engineering, University of Oklahoma

Authors and Affiliation: Prof. S.R. Gollahalli, Lesch Centennial Chair; Prof. R.N. Parthasarathy, Anadarko Petroleum Corporation Presidential Professor; and B.S. Dahifale Graduate Research Assistant

Previous studies indicate that when petroleum-based fuels are used with porous-media burners, NOx and CO emissions are reduced and combustion efficiency is improved. Since the properties of Canola Methyl Ester (CME) are different from those of petroleum-based fuels, research of combustion of CME blends with Jet A in a porous media burner was conducted. The combustion characteristics of CME-Jet A blends in volume percentages of 25%, 50% and 75% at four different equivalence ratios were studied. The different equivalence ratios were selected based on the stability of the flame. The operating conditions were varied by changing the fuel flow rate, while maintaining a constant flow rate of coflow and atomizing air. The combustion characteristics such as lift-off, extinction limits, global emissions, axial temperature profiles and radiative heat fractions were measured. Also, the flame appearance was recorded visually.

The results showed that the equivalence ratios of lift-off and extinction limits decreased with the addition of CME to Jet A. Also, the CO emission index decreased, whereas the NOx emission index increased with the CME content in the blend. As the equivalence ratio was increased, the CO2 concentration in the exhaust increased both for biofuels and Jet A, shows more complete combustion at higher equivalence ratios. Overall, it was found that the porous media burner was useful in reducing emissions and controlling the flame temperature with biofuels also.

T6: Measurement of Drag Coefficients of Biofuel Droplets in Free Fall
Presenter: Diana Martinez, Aerospace and Mechanical Engineering, University of Oklahoma

Authors and Affiliation: Professor Subramanyam R. Gollahalli, Lesch Centennial Chair; Professor Ramkumar N. Parthasarathy, Anadarko Petroleum Corporation Presidential Professor; Diana Martinez Graduate Research Assistant

Numerical simulation of biofuel sprays requires information of the drag coefficient of the drops in order to track the motion of the drops. The objective of this study is to compare the values of the drag coefficients of burning and non-burning droplets of three different fuels: petroleum-based No. 2 diesel fuel, canola methyl ester and soy methyl ester. The experimental set-up was designed to document the motion of free-falling drops of different sizes (ranging from 0.5 to 2.5 mm in diameter) in air at atmospheric pressure.

The temperature of the air needed to be controlled to keep the SME and CME drops burning, as they fell freely. Two flat ceramic heaters were used to heat the air (90°F to 150°F) between them; a K type thermocouple connected to a temperature controller and a relay switch were used to control the temperature of the heaters. Another K-type thermocouple positioned above the gap was used to anchor the droplets. The droplets were ignited by an external flame and underwent free fall through the gap of hot air between the heaters. The images of the free-falling burning droplets were captured using a Redlake MotionPro X3 camera with a 1280 x 1024 pixel resolution and a recording rate of 1000 frames per second. Analysis of the images was used to determine the drag coefficients of the burning and non-burning spray drops along their trajectories.
**T7: Soot Particle Analysis in Air-Flames of Canola Methyl Ester Biofuel and Diesel Fuel**  
**Presenter:** Wilson Merchan-Merchan, Aerospace and Mechanical Engineering, The University of Oklahoma  
**Authors and Affiliation:** W. Merchan-Merchan and S. Granados Sanmiguel; School of Aerospace and Mechanical Engineering The University of Oklahoma Norman, OK 73019-0390

This experimental investigation studies the soot formation of wick-generated open air-flames of Canola Methyl Ester (CME) biofuel and Diesel fuel. The microstructure of soot collected from selected flame locations is analyzed by combining the thermophoretic sampling technique and transmission electron microscopy (TEM). Examination of the evolution of soot particles along the axial streamline reveals the existence of two characteristic layers. For both flame types, nascent soot particles or soot precursor material are present in a region within the flame located just above the burner’s nozzle. The precursor particles undergo carbonization and agglomeration as they are driven through the flame volume forming the layer of mature soot. Analysis of the soot particle evolution, based on the morphology and size, was performed along the flame centerline for both cases. A strong correlation between soot morphology and local flame temperature is observed. High resolution TEM analysis performed on precursor or young and mature soot extracted from both flames reveals the presence of highly ordered carbon nanostructures.

**T8: Analysis of the Relative Fatty Acid Contents of Base and Acid Catalyzed Biodiesel**  
**Presenter:** Petar Petrov, Chemistry, University of Central Oklahoma  
**Authors and Affiliation:** Petrov, P. and McIntyre, E., University of Central Oklahoma

The two main methods for production of biodiesel, using either a base or an acid catalyst, vary in byproducts and fuel quality. This research compares the two methods through examination of the amounts of free fatty acids and the gel points of fuel produced via the two methods. Samples were produced on a small scale with both methods in a similar setting with store-bought canola oil. The base catalyzed reaction was performed with sodium hydroxide and methanol at 40°C for 30 minutes. The acid catalyzed reaction was performed with sulfuric acid and methanol at 70°C for 4 hours. Samples were collected, water washed, and separated into their component layers. Byproducts were discarded, while potential methyl ester (biodiesel) layers were analyzed for methyl ester content with a Gas Chromatograph Mass Spectrometer (GC-MS). The base catalyzed sample had a 10.4% overall yield of methyl esters while the acid catalyzed sample had a 7.54% overall yield. The samples were frozen and observed while melting to determine gel point. The gel point of the base catalyzed sample was -2°C, and of the acid catalyzed sample it was -6°C. These results indicate that base catalysis is preferred for small scale biodiesel production.

**T9: Condensation Reactions of Propanal over Ceria-Zirconia Mixed Oxide Catalysts**  
**Presenter:** Anirudhan Gangadharan, School of Chemical, Biological and Materials Engineering, University of Oklahoma  
**Authors and Affiliation:** Anirudhan Gangadharan, Min Shen, Tawan Sooknoi, Daniel E. Resasco and Richard G. Mallinson, Center for Biomass Refining and School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

Vapor phase aldol condensation and ketonization reactions of propanal were investigated over CexZr1-xO2 mixed oxides as a model reaction to produce gasoline range molecules from short aldehydes found in bio-oil mixtures. Several operating parameters were investigated. They include the type of carrier gas used (H2 or He) and the incorporation of acids and water in the feed. Propanal is converted to higher carbon chain oxygenates on CexZr1-xO2 by two pathways, aldol condensation and ketonization. The major products of these condensation reactions include 3-pentanone, 2-methyl-2-pentenal, 2-methylpentanal, 3-heptanone and 4-methyl-3-heptanone. It is proposed that the primary intermediate for the ketonization path is a surface carboxylate. The presence of acids in the feed inhibits the aldol condensation pathway by competitive adsorption that reduces the aldehyde conversion. Water also promotes ketonization and inhibits aldol condensation by increasing the concentration of surface hydroxyl groups that enhance the formation of surface carboxylates with the aldehyde. Hydrogen enhances cracking and production of light oxygenates and hydrocarbons. The light oxygenates may in turn be reincorporated into the reaction path, giving secondary products. However, the hydrocarbons do not react further. The analysis of the fresh and spent catalysts by XPS showed varying degrees of reduction of the oxide under different operating conditions and was in agreement with the reaction results. Changing the proportion of the parent oxides showed that increased Zr favored formation of aldol products while increased Ce favored ketonization. This occurred by shifting the balance of the acid-base properties of the active sites.
T10: Catalytic Upgrading of Switchgrass Pyrolysis Bio-oil Vapors over Ce0.5Zr0.5O2 Mixed Oxide Catalyst

Presenter: Jonathan Peters, School of Chemical, Biological, and Materials Engineering, University of Oklahoma

Authors and Affiliation: Jonathan E. Peters, Xiaohan Zhang, Trung T. Pham, Daniel Resasco and Richard G. Mallinson, Center for Biomass Refining, School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, 73019, USA

Catalytic upgrading of bio-oil from switchgrass pyrolysis was investigated over Ce0.5Zr0.5O2 mixed oxides to produce higher carbon chain molecules for use as fuel additives from short aldehydes and carboxylic acids found in bio-oil mixtures. The experiments were carried out in a single two-stage in situ process where the products from the pyrolysis reaction were fed directly to a fixed catalyst bed in a separate reactor in series with the pyrolysis reactor. The final products were condensed to the liquid phase and collected for analysis. GC by GC analysis of products shows evidence of catalytic activity. Acetic acid and propanoic acid found in the bio-oil were converted to acetone and 3-pentanone, respectively, when reacted over the catalyst. This is consistent with our work on model compounds that short aldehydes and carboxylic acids are converted to higher chain aldehydes and ketones by way of aldol condensation and ketonization over mixed oxides catalyst. Reacting over mixed oxides catalyst resulted in lower liquid yields from pyrolysis when compared to experiments without catalyst. The char yields remained the same while the gas yields, by difference, appear to have increased under these conditions.

T11: Selective Deoxygenation of Furfuraldehyde on Bimetallic Pd-Cu Catalysts

Presenter: Trung Pham, Chemical Engineering, University of Oklahoma

Authors and Affiliation: Trung T Pham, Surapas Sitthisa, Lance L Lobban, Daniel E Resasco and Richard G Mallinson. Center for Biomass Refining and School of Chemical, Biological and Materials Engineering University of Oklahoma 100 Boyd St, T-335 Norman, OK 73019

Bimetallic Pd-Cu catalysts have been studied for the hydrogenation and deoxygenation of 2-methylpentanal. Compared to Pd catalysts, Pd-Cu shows a decrease in conversion of 2-methylpentanal. At low W/F, 5% Pd-2.5% Cu/SiO2 exhibits high selectivity for hydrogenation to 2-methyl-pentanol and substantially reduced decarbonylation activity compared with pure 5% Pd/SiO2. The bimetallic shows that the ratio of etherification of the alcohol product with the 2-methylpentanal is much greater than for Pd alone, since the parallel decarbonylation is reduced. Compared at the same 25 % conversion of 2-methylpentanal, the product yield ratio of dimethylpentyl ether/pentane is 4 times higher on the 5% Pd-2.5% Cu/SiO2 than on the 5% Pd/SiO2. The addition of Cu decreases the number of \( \eta_2 \) sites that are needed for both decarbonylation and etherification. However, the bimetallic maintains good ether selectivity due to its ability to readily hydrogenate the aldehyde to the intermediate alcohol and continue to form the required surface alkoxide in proximity to the remaining \( \eta^* \) sites.

T12: Reactions of 2-Methylpentanal on Bimetallic Pd-Cu Catalysts

Presenter: Trung Pham, Chemical Engineering, University of Oklahoma

Authors and Affiliation: Trung T Pham, Surapas Sitthisa, Lance L Lobban, Daniel E Resasco and Richard G Mallinson. Center for Biomass Refining and School of Chemical, Biological and Materials Engineering University of Oklahoma 100 Boyd St, T-335 Norman, OK 73019

Bimetallic Pd-Cu catalysts have been studied for the hydrogenation and deoxygenation of 2-methylpentanal. Compared to Pd catalysts, Pd-Cu shows a decrease in conversion of 2-methylpentanal. At low W/F, 5% Pd-2.5% Cu/SiO2 exhibits high selectivity for hydrogenation to 2-methyl-pentanol and substantially reduced decarbonylation activity compared with pure 5% Pd/SiO2. The bimetallic shows that the ratio of etherification of the alcohol product with the 2-methylpentanal is much greater than for Pd alone, since the parallel decarbonylation is reduced. Compared at the same 25 % conversion of 2-methylpentanal, the product yield ratio of dimethylpentyl ether/pentane is 4 times higher on the 5% Pd-2.5% Cu/SiO2 than on the 5% Pd/SiO2. The addition of Cu decreases the number of \( \eta_2 \) sites that are needed for both decarbonylation and etherification. However, the bimetallic maintains good ether selectivity due to its ability to readily hydrogenate the aldehyde to the intermediate alcohol and continue to form the required surface alkoxide in proximity to the remaining \( \eta^* \) sites.
8:30 AM - 11:40 AM Sooner B

**S3: Chemical Education/POGIL**
Chair and Presider: *Michael Abraham* (Chemistry & Biochemistry, The University of Oklahoma)

**ABSTRACTS**

8:30 T13 Adapting a Methodology for Documenting Collective Growth to an Undergraduate Physical Chemistry Class

8:50 T14 A New Approach to General Chemistry: Switching from Topics to Questions

9:10 T15 Teaching Chemistry with Visualization

9:30 T16 Inquiry in Large Class Settings: Before, During, and After Class Activities

9:50 DISCUSSION

10:00 BREAK

10:20 T17 POGIL in a Large Enrollment Organic Chemistry I Course

10:40 T18 Getting from "Wow!" to "Aha!": Using POGIL to Spur Learning From Demonstrations

11:00 T19 Math as a Second Language: A New Model for Math Literacy in the Science Classroom

11:20 T20 Use of a Spreadsheet to Calculate the Net Charge of Peptides and Proteins as a Function of pH: an Alternative to Using "Canned" Programs to Estimate the Isoelectric Point (pI) of These Important Biomolecules

11:40 DISCUSSION

**T13: Adapting a Methodology for Documenting Collective Growth to an Undergraduate Physical Chemistry Class**
*Presenter*: Renee Cole, Biochemistry, Chemistry & Physics, University of Central Missouri

*Authors and Affiliation*: Renee Cole, University of Central Missouri; Marey Towns, Purdue University; Chris Rasmussen, San Diego State University; Nicole Becker, Purdue University; George Sweeney, San Diego State University; Megan Wawro, San Diego State University

Physical Chemistry is a subject that uses mathematical inscriptions to carry chemical meaning. In order to gain understanding, both curricular and pedagogical, of how students build an understanding of mathematical inscriptions that are used in chemistry, it is necessary to document student reasoning and classroom practices. A three-phase approach grounded in Toulmin's argumentation scheme was developed to trace the growth of ideas in an inquiry mathematics classroom. This method of documenting collective production of meaning was adapted for use in analyzing an inquiry-oriented physical chemistry classroom. The difference in classroom structure between mathematics and physical chemistry necessitated modifications to the application of the methodology, but the analysis provided empirical evidence for common themes that define physical chemistry classroom practices. This evidence will be presented along with the implications for instructional design and teaching.

**T14: A New Approach to General Chemistry: Switching from Topics to Questions**
*Presenter*: Vicente Talanquer, Chemistry and Biochemistry, University of Arizona

*Authors and Affiliation*: Vicente Talanquer and John Pollard. Department of Chemistry and Biochemistry, University of Arizona.

Despite multiple calls for reform, the curriculum for first-year college chemistry at many universities across the world is still mostly fact-based and encyclopedic, built upon a collection of isolated topics, oriented too much towards the perceived needs of chemistry majors, focused too much on abstract concepts and algorithmic problem solving, and detached from the practices, ways of thinking, and applications of both chemistry research and chemistry education research in the 21st century. This paper describes an alternative way of conceptualizing the introductory chemistry curriculum for science and engineering majors by shifting the focus from learning chemistry as a body of knowledge to understanding chemistry as a way of thinking and answering questions. The central goals of our new curriculum are to: promote deeper conceptual understanding of a minimum core of fundamental ideas instead of superficial coverage of multiple topics; connect core ideas between the course units by following well-defined learning progressions; introduce students to modern ways of thinking and problem-solving in chemistry; and involve students in realistic decision-making and problem-solving activities.

**T15: Teaching Chemistry with Visualization**
*Presenter*: Vickie Williamson, Chemistry, Texas A & M University

Visualization techniques in the chemistry classroom are used to promote more expert-like mental models in students. A chemist can visualize a chemical reaction on the macroscopic level, what the reaction will look like to the human eye in the laboratory, and on the particulate level, what changes are taking place in the atoms and molecules. Techniques to help students create these mental images of the macroscopic level include laboratory simulations and demonstrations. Techniques that promote mental images on the particulate level include physical models, role-playing, fixed computer models, dynamic computer animations, student-generated drawings/animations, and interactive computer models. This paper reviews chemical education research findings on these techniques. Implementation strategies for each technique will be discussed.
demonstrations. Several examples will be presented in
POGIL is used as a means of creating careful
they are merely entertained by them. In this work
whether students learn from these demonstrations or if
of General Chemistry instruction. However, it is unclear
Demonstrations are a common and popular component
Oklahoma City, OK

Authors and Affiliation: Michael R Abraham
Department of Chemistry and Biochemistry University
of Oklahoma Norman, Oklahoma; John I Gelder
Department of Chemistry Oklahoma State University
Stillwater, Oklahoma; Tomas J. Greenbowe Department
of Chemistry Iowa State University Ames, Iowa

An inquiry based instructional strategy can be used to
guide the development of instructional materials. Details of a research-based, inquiry-oriented instructional
strategy (the Learning Cycle Approach) will be
discussed. Examples of instructional materials for
“before”, “during”, and “after” general chemistry class
meetings based on this strategy will be presented.

T17: POGIL in a Large Enrollment Organic
Chemistry I Course
Presenter: Mark Morvant, Chemistry & Biochemistry,
University of Oklahoma
Authors and Affiliation: Mark C. Morvant University
of Oklahoma

During the Fall 2009 semester, the author taught two
sections of the Organic Chemistry I, one of the sections
using a traditional lecture format and the other using
POGIL. The enrollments for the sections were 275 and
240 students in the “lecture” and POGIL sections,
respectively. The presentation will include the structure
of the sections, the author’s impression of the
implementation, the students’ attitudes toward the
formats as indicated in a student survey, and the initial
results from the comparison of the students’ performance
in the two sections.

T18: Getting from "Wow!" to "Aha!": Using POGIL
to Spur Learning from Demonstrations
Presenter: Stephen Prilliman, Chemistry, Oklahoma
City University
Authors and Affiliation: Oklahoma City University,
Oklahoma City, OK

Demonstrations are a common and popular component
of General Chemistry instruction. However, it is unclear
whether students learn from these demonstrations or if
they are merely entertained by them. In this work
POGIL is used as a means of creating careful
observation, investigation and discussion of classroom
demonstrations. Several examples will be presented in
which a demonstration has served as the observational
model in a POGIL activity. Such POGIL-structured
demonstrations could serve as a means of creating
discrepant events that force to learners to confront
misconceptions and create new internal models to
understand their observations.

T19: Math as a Second Language: A New Model For
Math Literacy in the Science Classroom
Presenter: Benjamin Sandler, Biochemistry, Oklahoma
State University
Authors and Affiliation: Benjamin Sandler, Department
of Biochemistry, Oklahoma State University

Students in the science classroom must be able to
connect the physical reality of a system with its
mathematical description. But, traditional, derivation-
based teaching connects the two with lengthy and
abstract mathematical manipulations that do little to
provide students with an immediate, intuitive
understanding of the meaning of the equations. The
Math as a Second Language (MSL) methodology uses a
range of techniques to teach students to read equations as
descriptions of physical systems, as if they were reading
English text. For example, equations are broken down into “vocabulary words” which describe different aspects
of the physical system’s behavior. Students are taught to
associate these “words” with intuitively accessible
mental pictures that express aspects of the physical
system’s behavior. When these “words” recur across
different equations, students can recognize them as
describing similar qualities of different systems. The
effectiveness of MSL was tested in a junior-level
biochemistry class and a senior-level physical
biochemistry class using mixed methods. Student
response to MSL is enthusiastic. The techniques of
MSL, its effect on student performance, and future
directions will be discussed.

T20: Use of a Spreadsheet to Calculate the Net
Charge of Peptides and Proteins as a Function of pH:
an Alternative to Using "Canned" Programs to
Estimate the Isoelectric Point (pI) of These Important
Biomolecules
Presenter: Paul Sims, Chemistry & Biochemistry, The
University of Oklahoma
Authors and Affiliation: University of Oklahoma

An approach is presented that utilizes a spreadsheet to
allow students to explore different means of calculating
and visualizing how the charge on peptides and proteins
varies as a function of pH. In particular, the concept of
isolectric point (pI) is developed to allow students to
compare the results of their spreadsheet calculations with
those of computer programs that are freely available on
the Internet and are designed to calculate the same
parameter. Such comparisons allow students to explore
the underlying assumptions of their model (and the likely
assumptions of the computer programs) and to speculate
on ways in which their model might be improved. A
discussion of the oligomeric protein hemoglobin is
included to show the limitations of the computer
programs and to show how the spreadsheet approach can
be adapted to treat satisfactorily this important protein.
8:30 AM - 10:00 AM Ballroom A

S4: Nanotechnology - Biological Applications

Chair and Presider: Donna Nelson (Chemistry & Biochemistry, The University of Oklahoma)

8:30 T21 Targeted Nano-Biological Probes for Tumor Markers Visualized by Molecular Magnetic Resonance Imaging (mMRI)

8:50 T22 Novel Magnetic Nanoparticles for Gene Delivery in Mesenchymal Stem Cells

9:10 T23 Using Fluorescent Nanoparticles for Transfection of Plant Cells

9:30 T24 Virus Enabled Photosensitizer for Photodynamic Therapy in Breast Cancer Cells

T21: Targeted Nano-Biological Probes for Tumor Markers Visualized by Molecular Magnetic Resonance Imaging (mMRI)

Presenter: Rheal Towner, Advanced Magnetic Resonance Center, Oklahoma Medical Research Foundation

Authors and Affiliation: Authors: Rheal A. Towner,1 Nataliya Smith,1 Debra Saunders,1 Sabrina Doblas,1 Ting He,1 Yasuko Asano,1 Charles E. Seeley,1 Robert Silasi-Mansat,2 and Florea Lupu2 Affiliations: 1) Advanced Magnetic Resonance Center, and 2) Cardiovascular Biology, Oklahoma Medical Research Foundation, Oklahoma City, OK 73104, and 3) NanoBioMagnetics Inc., Edmond OK 73034

Targeted nanobiological probes were used to establish in vivo levels of cancer biomarkers in a rodent model for gliomas, a primary brain cancer. The levels of c-Met, a tyrosine kinase receptor for the hepatocyte growth- or scatter-factor, and of the vascular endothelial growth factor receptor 2 (VEGF-R2), an angiogenetic factor, are both elevated during tumor development. This study involved the development and assessment of novel molecular MRI (mMRI) probes for the in vivo detection of c-Met and VEGF-R2 in an experimental rodent C6 glioma model. The molecular targeting agent we used in our study incorporated a magnetite-based dextran-coated nanoparticle backbone covalently bound to an anti-Met antibody (Ab). We used molecular MRI (mMRI) with either an anti-Met or an anti-VEGF-R2 probe to detect in vivo c-Met or VEGF-R2 levels as molecular markers for gliomas. Tumor regions were compared to normal tissue, and found to significantly (p<0.05) decrease MR signal intensity and T2 relaxation in tumors. Non-immune non-specific normal rat IgG coupled to the dextran-coated nanoparticles was used as a control contrast agent. c-Met or VEGF-R2 levels in tumor tissues were confirmed in Western blots and via immunohistochemistry (IHC). Prussian blue staining of brain tissues previously administered the targeted nanobiological probes was used to confirm the presence of the iron oxide-based nanoparticles in tumors. Targeted-nanobiological probes can be useful tools for the diagnosis of specific cancers and/or characterizing tumor malignancy.

T22: Novel Magnetic Nanoparticles for Gene Delivery in Mesenchymal Stem Cells

Presenter: Ananta Ayyagari, Department of Chemistry and Biochemistry, University of Oklahoma

Authors and Affiliation: Ananta Laxmi Ayyagari, Haibao Zhu, DongDong Wang and Chuanbin Mao Department of Chemistry and Biochemistry University of Oklahoma, Norman,OK

Mesenchymal stem cells (MSCs) have been proposed as an attractive target for the gene therapy owing to their ability to promote the regeneration of mesenchymal tissues such as bone, cartilage, muscle, ligament, tendon etc. MSCs undergo rapid division and are readily transducible with integrating vectors and above all maintain transgene expression in vitro and in vivo without any effect on its multipotentiality. The need for newer safe and effective gene delivery methods have resulted in tremendous efforts in the preparation and characterization of novel non viral vectors. Among the plethora of non viral vectors, cationic lipids mediated gene delivery has been vastly studied and has proved to be least toxic with high transfection efficiency. In recent times, magnetofection, the use of magnetic field to increase delivery of gene is reaching new heights. Towards this end, we hypothesize a novel magnetic particle conjugated with DNA (PCR fragments) via a disulfide bond would effectively transfect the cells. The rationale behind the design of such a conjugate is the cleavage of disulfide bond in the presence of glutathione inside the cells facilitating easy delivery of the DNA. Moreover, the use of DNA (PCR Product) fragments instead of a plasmid DNA would lead to higher nuclear pore uptake through diffusion. The magnetic particle-DNA complex would also be encapsulated inside a cationic lipid bilayer membrane to protect it from the nuclease degradation. The target specificity to the mesenchymal stem cells would be studied by incorporating the desired protein on the cationic liposomal membrane.
T23: Using Fluorescent Nanoparticles for Transfection of Plant Cells

Presenter: Jeanmarie Verchot-Lubicz, Entomology and Plant Pathology, Oklahoma State University

Authors and Affiliation: Jeanmarie Verchot-Lubicz, Oklahoma State University; Asitha DeSilva, Oklahoma State University

We have conducted proof of concept experiments to determine if fluorescent conjugated polymer nanoparticles (CPNs) can be delivered to plant tissues. The CPNs were developed for the labeling and delivery of biological interests. CPNs have the potential to be used for delivery of RNA silencing signals, to study transport systems, and to study cytoplasmic streaming. Current research has shown that tobacco protoplasts can take up CPNs with no detectible toxicity. Fluorescent CPNs can also be used to study cellular dynamics and intercellular transport. Fluorescent CPNs can be used to deliver small interfering RNAs (siRNAs) to cells to knock out expression of targeted genes. We are working to expand the applications of this technology.

T24: Virus Enabled Photosensitizer for Photodynamic Therapy in Breast Cancer Cells

Presenter: Naveen Gandra, Chemistry and Biochemistry, University of Oklahoma

Authors and Affiliation: Naveen Gandra, Gopal Abbineni, and Chuanbin Mao* University of Oklahoma, Department of Chemistry and Biochemistry, 620 Parrington Oval, Norman, OK 73019

Photodynamic therapy (PDT) is a light activated treatment procedure for several types of cancers and other diseases. PDT requires the preferential accumulation of photosensitizer in malignant tumor, followed by the irradiation with appropriate laser light that can generate the cytotoxic singlet oxygen (\(1^\text{O}_2\)) and thereby resulting in death of the malignant cells via apoptosis and/or necrosis. Currently, PDT is widely being used worldwide for macular degeneration and destruction of certain kind of solid tumors. However, the use of PDT is limited by the lack of long wavelength absorption which limits the light penetration in the cells, poor solubility, and lack of selectivity for targeted tissues. Our group has been using the genetically engineered viruses for several applications ranging from biological sensing to drug delivery. Here, we are using an engineered fd filamentous bacteriophage as a carrier to selectively deliver into breast cancer cells (SKBR3). Our novel phage-conjugated sensitizer integrates all the properties of traditional photosensitizer with selectivity, leading to the development of third generation photosensitizers for photodynamic therapy.
**S5: Nuclear Magnetic Resonance**  
Chair and Presider: Susan Schroeder  
(Chemistry and Biochemistry, University of Oklahoma)

8:30 T25 Tying up the Ends: Recognition of ssDNA at Telomeres

Presenter: Deborah Wuttke, Chemistry and Biochemistry, University of Colorado

Authors and Affiliation: Deborah S. Wuttke, Johnny E. Croy, Aimee M. Eldridge, Nicole E. Grimm, Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, USA, 80309-0215

Telomeres, the nucleoprotein complexes at the ends of chromosomes, mediate essential functions required for genomic stability, including protection of the chromosome ends from inappropriate recognition by the DNA damage-sensing machinery and ensuring complete chromosomal replication. Loss of proper telomere function is devastating to the cell due to the introduction of chromosomal abnormalities such as end resection, end-to-end fusions, and aberrant DNA recombination. In addition, loss of telomere replication by the reverse-transcriptase telomerase results in the gradual erosion of telomeric DNA eventually resulting in cellular senescence. At the core of these critical telomere functions are a family of proteins that bind the universally conserved 3’ single-strand DNA (ssDNA) G-rich overhang at the ends of telomeres with high affinity and exquisite specificity. In higher eukaryotes, the Pot1 proteins recognize and bind the single-stranded overhang and regulate both telomere end-protection and telomerase activity, while in the budding yeast, the essential ssDNA-binding protein Cdc13 performs these functions.

In order to better understand how ssDNA recognition is linked to these two essential functions, we have investigated the structural and dynamic features that guide the recognition of single-stranded DNA within this family using NMR strategies. Based on these results, we have discovered how each protein has evolutionarily adapted to recognize the features of its unique ssDNA substrate. Furthermore, we have discovered a novel mechanism of structural accommodation where the flexible nature of both protein and ssDNA substrate are exploited to allow binding in multiple thermodynamically equivalent conformations.

We gratefully acknowledge NIH (GM059414 and GM068928) and NSF (MCB0617956) for funding.

T26: NMR Structure of phi29 Prohead RNA E-loop Hairpin

Presenter: Steven Harris, Chemistry/Biochemistry, University of Oklahoma

Authors and Affiliation: Steven Harris and Dr. Susan J. Schroeder, Department of Chemistry and Biochemistry, University of Oklahoma

Bacillus subtilis phage phi29 packaging motor requires prohead RNA for genome encapsidation. The NMR structure of the prohead RNA E-loop hairpin, r(5'AUUGAGUU), and MC-SYM predictions for prohead RNA E-loops provide a basis for comparative analysis of hairpin structures in prohead and ribosomal RNA. All the hairpins contain a U-turn motif but differ in the first noncanonical pair and backbone orientation. These structures provide benchmarks for further improvements in RNA structure predictions from sequence.

T27: NMR Studies of Human MID1, a Novel E3 Ligase Targeting Protein Phosphatase 2A

Presenter: Michael Massiah, Biochemistry and Molecular Biology, Oklahoma State University

Authors and Affiliation: Michael A. Massiah, Department of Biochemistry and Molecular Biology, Oklahoma State University, Stillwater OK 74078

Human midline-1 (MID1) is a microtubule-associated TRIM protein that is hypothesized to target the catalytic subunit of protein phosphatase 2A (PP2Ac) for degradation. MID1 first bind alpha4, a novel regulatory domain of PP2Ac that either recruits or has already bound PP2Ac. MID1 consists of three non-homologous N-terminal zinc-binding domains (RING, Bbox1 and Bbox2), followed by a coiled-coil (RBC) domain. As with proteins with RING domains, MID1 RING domain is assumed to possess the ubiquitin E3 ligase activity that facilitates the ubiquitination of PP2Ac. Our structures of the Bbox1 and Bbox2 domains, individually and in tandem, reveal that they may also function as E3 ligases. Indeed based on our NMR structures, new functional models of MID1 are emerging.
NMR determination of protein structure is essential for elucidating function. Compared to X-ray crystallography, NMR has the potential to show structure in an aqueous environment that better models in vivo conditions. However, NMR has size limitations and protein solubility issues not encountered in crystallization. The Midline-1 (MID1) protein is an important protein in embryogenesis. Mutations of MID1 are associated with X-linked Opitz Syndrome characterized by midline anomalies such as a cleft lip, wide spaced eyes, heart and brain defects, and genitalia malformation. Full length MID1 is not amenable for structural study. MID1 consists of a Fibronectin type 3 (FN3) domain the structure and function of which are unknown. Here we present the NMR studies of FN3 and the RING domain that show that these small proteins polymerize in solution as demonstrated by HSQC spectroscopy. Dynamic light scattering confirmed that the GB1-FN3 forms monodisperse aggregate with an estimated size of 25 monomers.

The interactions in the poly(vinyl acetate) and dipropylene glycol) dibenzoate (a plasticizer) system were studied with deuterium NMR. Both the polymer and plasticizer were separately labeled and used to follow the dynamics of each. It was found that in bulk, the temperature for the onset of molecular motion, that narrows the deuterium NMR quadrupole pattern, was lower for the plasticizer than the polymer. For systems where the polymer (and plasticizer) were adsorbed on silica, the polymer mobility increased with larger amounts of polymer adsorbed and plasticizer added. In contrast, the mobility of the plasticizer was highest for the sample with the smallest amount of polymer adsorbed. This effect is ascribed to the exclusion of the plasticizer in the polymers adsorbed at low adsorbed amounts.

An effective means of studying biological metal chemistry is through the use of cadmium NMR to probe the interaction between biomolecules, such as proteins and peptides, with divalent metals, such as zinc, copper, magnesium, or calcium. Gram-positive bacteria, such as S. aureus and B. subtilis, have peptidoglycan cell walls that contain teichoic acids, a poly(phosphodiester) biopolymer used for, among other things, metal chelation. Previous solid-state NMR and XAFS studies have shown that the cadmium ion binds in a bidentate manner to the phosphoryl centers of the dried teichoic acid backbone at physiological pH. However, current studies indicate that, when hydrated and at the low concentrations typically found in nature, the cadmium ions and phosphoryl sites interact through an extended solvent-separated ion pairing. These data reveal two unequal P–Cd interactions at distances of 4.2 and 4.9 Å set approximately 180° from each other in a linear arrangement.
**T32: Multi-Receiver NMR**

**Presenter:** Yasvir Tesiram, Advanced Magnetic Resonance Center, Oklahoma Medical Research Foundation

**Authors and Affiliation:** Oklahoma Medical Research Foundation, 825 NE 13th St, OKC, OK, 73104

Recently multi-receive nuclear magnetic resonance (NMR) spectroscopy was described wherein a number of standard NMR experiments were combined into a single experiment allowing for complete structure determination of a small molecule\(^1\)^\(^2\). In essence this advancement in parallel reception of the NMR signal is promising from the point of view of overcoming limitations where separate NMR experiments are usually acquired. In this spectrometer there are two or more broad-band receivers and one proton receiver. If combined with triple axis field gradients, simultaneous imaging and spectroscopy is also possible. The advantage of such spectrometers include true simultaneous reception of multiple frequencies and easier manipulation of data acquisition from within pulse sequence programs as opposed to time inefficient macro driven acquisition schemes. In addition re-cabling of various spectrometer channels is not required even if switching from decoupling mode to direct observe mode. In the simplest realization of an advantage, since time must inevitably be spent for accumulating signal of insensitive nuclei (e.g. \(^{13}\)C), the signal to noise ratio (SNR) of more sensitive nuclei (e.g. \(^1\)H) are dramatically improved if collected simultaneously or even sequentially. In fields such as metabolomics, previously ignored resonances constrained by SNR limits suddenly become accessible. The detection of these metabolites in one single experiment combined with a potential structural identity are of great diagnostic potential in disease especially in understanding mechanisms of disease and incorporation into systems biology models. Other applications may include reaction kinetics experiments of labeled compounds where insensitive nuclei may be simultaneously detected rather than indirectly. Examples of these experiments will be presented. In addition, collection of 2D homo and heteronuclear correlation spectra will also be presented.

The disadvantage of a multi-receive spectrometer at the current time is that there are very few new pulse sequences and experiments with untenable advantage over existing methods. In looking for time efficiencies in NMR spectroscopy a number of limitations are immediately recognized. In the first instance it is not possible to decouple and acquire the same nucleus. Thus this emerging field is open for research into new and exciting techniques from a pulse programming perspective and spin physics. For example, during an evolution period such as those required for polarization transfer all single quantum states at any point in a pulse sequence are observable and provide valuable information on spin dynamics (or rather "state"). The observation of these states is of potential importance in quantum computers, but the collection of such signals requires a number of pulse sequence elements to be carefully synchronized. Preliminary observations and design methods will also be presented.


8:30 AM - 11:40 AM Sooner A

S6: X-Ray Crystallography

Chair and Presider: Leonard Thomas
(Chemistry & Biochemistry, The University of Oklahoma)

8:30 T33 The Distal Pocket Histidine Residue in Horse Heart Myoglobin Directs the O-Binding Mode of Nitrite to the Heme Iron

8:50 T34 Understanding the Architecture and Assembly of Large Double-Stranded DNA Icosahedral Viruses

9:10 T35 Crystal Structure of an Eight-Base Pair Fragment from a U-tail Helix Domain from RNA Editing Complexes in Trypanosoma brucei

9:30 T36 Structural Biology Study of Biosynthesis of Plant Natural Products

10:00 BREAK

10:20 T37 X-Ray Crystal Structure of Acetyl Esterase from Escherichia coli

10:40 T38 Rejuvenating a Classic Antimicrobial Target for Today’s Anti-Bacterial Needs

11:00 T39 IL18 & IL18BP in Autoimmune and Infectious Diseases

11:20 DISCUSSION

T33: The Distal Pocket Histidine Residue in Horse Heart Myoglobin Directs the O-Binding Mode of Nitrite to the Heme Iron

**Presenter:** Jun Yi, Chemistry and Biochemistry, University of Oklahoma

**Authors and Affiliation:** Jun Yi, George B. Richter-Addo, Department of Chemistry and Biochemistry, University of Oklahoma

Nitrite is ubiquitous in the environment, and its reduction to nitric oxide (NO) by denitrifying metalloenzymes is an important component of the global nitrogen cycle. However, nitrite has commonly been viewed as a physiological “dead end” product of NO oxidation. It is now known that the ferrous heme protein myoglobin (Mb) reduces nitrite to NO under hypoxic conditions. We demonstrate here that the single H-bonding distal pocket histidine residue (His64) of horse heart metMbIII directs the O-binding mode of nitrite to the heme iron.

X-ray crystal structures were determined for the mutant proteins metMbIII H64V (2.0 Å resolution) and its nitrite ion adduct metMbIII-H64V-nitrite (1.95 Å resolution), and metMbIII H64V/V67R (1.9 Å resolution) and its nitrite ion adduct metMbIII-H64V/V67R-nitrite (2.0 Å resolution). In contrast to the known structures of wild type hh metMbIII, no axial H2O is evident in either of the metMbIII mutant structures. By removing the single H-bonding His64 residue in Mb, the binding mode of nitrite switches from the nitrito (O-binding) form in the wt protein to a weakly bound nitro (N-binding) form in the H64V mutant. Reintroducing a H-bonding residue in the H64V/V67R double mutant restores the O-binding mode of nitrite.

T34: Understanding the Architecture and Assembly of Large Double-Stranded DNA Icosahedral Viruses

**Presenter:** Stacy Benson, Chemistry, Oklahoma State University

**Authors and Affiliation:** Stacy D. Benson Department of Chemistry, Oklahoma State University, 107 Physical Sciences, Stillwater, OK, 74078

The number of virus species is predicted to be an order of magnitude larger than the number of all other species combined. Most viruses have not been investigated or even discovered. How can we make sense of this large number of viral types? My group is looking at the characteristics of large, double-stranded DNA viruses, which is just one subsection of the virus species. The X-ray crystallographic structure of the main coat protein of bacteriophage PRD1, P3, has revealed a fold similar to the major coat protein, hexon, of the human adenovirus. Further structural studies, using cryo-electron microscopy and X-ray crystallography, have shown that the architecture of these two viruses is very similar. Using bioinformatics and literature searches, additional viral families have been identified that are expected to have similar major coat protein folds and viral architectures, suggesting that these viruses could all represent a viral lineage. It is expected that this group of viruses also use similar mechanisms for packaging their genome into empty capsids. Structural studies of select ATPases, which supplies the needed energy for packaging, from representative viruses have begun.
**T35: Crystal Structure of an Eight-Base Pair Fragment from a U-tail Helix Domain from RNA Editing Complexes in Trypanosoma brucei**

**Presenter:** Blaine Mooers, Biochemistry and Molecular Biology, University of Oklahoma Health Sciences Center  
**Authors and Affiliation:** Blaine H. M. Mooers, Dept. of Biochemistry and Molecular Biology, OUHSC  
Amritanshu Singh, Dept. of Biochemistry and Molecular Biology, OUHSC

Hundreds of guide RNAs (gRNAs) hybridize in trans with their target pre-mRNAs during uridiylate (U) insertion/deletion editing of pre-mRNAs at thousands of sites in the mitochondrion of trypanosomes. The 3’ end of the gRNA has about 5-25 uninterrupted Us (the U-tail) that are added after transcription. The U-tail binds to the purine-rich pre-mRNA upstream from the editing sites. The resulting structural domain is a double-stranded helix (the U-helix) with a high frequency of G•U wobble base pairs. The function of the U-helix remains an open biological question. To gain insight into the function of the U-helix through its structure, we crystallized an eight base-pair fragment of the U-helix formed by the gRNA gA6-14 and the mRNA transcript A6 for subunit 6 of the mitochondrial ATP synthase complex from Trypanosoma brucei. Two identical U-helices were fused head-to-head to avoid end-on-end disorder in the crystal lattice. The 1.37 Å crystal structure of the U-helix fragment varied in a base sequence dependent manner when compared to the 1.52 Å crystal structure of a RNA with the G•U wobble base pairs replaced with GC Watson-Crick base pairs. The helical variation may aid strand separation at the editing site during editing reactions.

**T36: Structural Biology Study of Biosynthesis of Plant Natural Products**

**Presenter:** Hui Shao, Plant Biology Division, The Samuel Roberts Noble Foundation  
**Authors and Affiliation:** Hui Shao, Lenong Li, Luis L. Escamilla-Trevino, Luzia Modolo, Lahoucine Achnine, Jack W. Blount, Xianzhi He, Richard A. Dixon and Xiaoqiang Wang. Plant Biology Division, Samuel Roberts Noble Foundation, 2510 Sam Noble Parkway, Ardmore, OK 73401

Plants synthesize huge numbers of natural products to accommodate environmental challenges and protect against attack from microorganisms and herbivores. Many of these plant natural products can be used for the benefit of human and animal health. The biosynthesis of plant natural products is very complex with many enzymes involved in many different chemical reactions including reduction, oxidation, hydroxylation, dehydration, glycosylation, methylation, condensation and cyclization. We are working on three types of enzymes involved in plant natural product biosynthesis, including reductases involved in reduction reactions, glycosyltransferases for glycosylation, and cytochrome P450s involved in hydroxylation and dehydration. We determined the structures of two NADPH-dependent reductases, three uridine diphosphate glycosyltransferases, and one cytochrome P450 enzyme. These enzyme structures provide essential insights into their structure-function relationships and catalytic mechanisms in the complex biosynthetic processes, and also provide a guide to manipulate the enzymes and the biosynthesis of natural products in plants for improving plant, animal and human health.

**T37: X-Ray Crystal Structure of Acetyl Esterase from Escherichia coli**

**Presenter:** Mamiko Nishida, Chemistry, Oklahoma State University  
**Authors and Affiliation:** Mamiko Nishida and Stacy D. Benson, Department of Chemistry, Oklahoma State University, 107 Physical Sciences, Stillwater OK 74078

Aes is an Escherichia coli protein consisting of 319 amino acids. It acts as an acetyl esterase and belongs to the family of hormone sensitive lipases (HSL). Aes down-regulates MalT that is the transcriptional activator of the maltose regulon in E. coli. Moreover, a recent study suggests an interaction between Aes and α-galactosidase. The aim of this study is to investigate the structure and function of Aes that plays essential roles in the regulation of carbohydrate metabolism in E. coli. X-ray crystallography reveals Aes has an α/β fold, typical to HSL, and functions as a serine hydrolase with the catalytic triad of Ser165, Asp262, and His292. In this presentation, structure determination of Aes and its function will be discussed.
T38: Rejuvenating a Classic Antimicrobial Target for Today's Anti-Bacterial Needs  
**Presenter:** Christina Bourne, Veterinary Pathobiology, Oklahoma State University  
**Authors and Affiliation:** Christina R. Bourne1, Richard A. Bunce2, Esther W. Barrow1, Philip C. Bourne1, K. Darrell Berlin1, William W. Barrow1; 1Center for Veterinary Health Sciences, Dept. of Veterinary Pathobiology, and 2Department of Chemistry, Oklahoma State University

The infectious burden on human health has steadily increased due largely to the emergence of drug-resistance, causing a commensurate increase in the necessity for new antimicrobial treatments. Despite a previously robust development pipeline, new antibiotics are no longer given priority in most drug development programs. We have re-examined targets in the folate pathway and focused on inhibition of dihydrofolate reductase (DHFR). DHFR is required for nucleic acid metabolism and is inhibited by folate analogs such as methotrexate (anti-cancer), pyrimethamine (anti-malarial) and trimethoprim (antibiotic). We have studied analogs containing an acryloyl linker and large dihydrophthalazine moiety for activity against microorganisms including *B. anthracis* and *S. aureus*. We find potent inhibition exemplified by low minimum inhibitory concentrations (MIC’s) ≤ 16 μg / mL and IC₅₀ values in the low nM range. We have focused on a derivative with a propyl group extending from the dihydrophthalazine, termed RAB1. This derivative displays broad spectrum antimicrobial activity and is especially potent against *S. aureus*, including drug resistant strains (MRSA/VRSA). Binding of RAB1 has been visualized in co-crystal structures with DHFR enzymes from *B. anthracis* and *S. aureus*. This has revealed previously unappreciated details in the volume of bacterial DHFR binding sites and highlighted a unique surface cavity in *S. aureus* DHFR that is susceptible to inhibitor binding. These structures have also allowed comparisons with human DHFR and confirmed the smaller size of human DHFR’s binding site. Current details are expected to contribute to future modifications of dihydrophthalazine derivatives, which now have demonstrated performance as important future antibiotics.

T39: IL18 & IL18BP in Autoimmune and Infectious Diseases  
**Presenter:** Junpeng Deng, Biochemistry and Molecular Biology, Oklahoma State University  
**Authors and Affiliation:** Brian Krumm1, Xiangzhi Meng,2 Yan Xiang2 and Junpeng Deng.1 1. Department of Biochemistry and Molecular Biology, Oklahoma State University, Stillwater, OK 2. Department of Microbiology and Immunology, UTHSCSA, San Antonio, TX

IL-18 plays a central role in inflammation and development of the adaptive immune response. Initially described as a potent inducer of IFN-gamma, IL-18 also induces other pro-inflammatory cytokines and chemokines, activates NK-cell activity and helps drive development of type-1 T-cells. IL-18 is an important mediator in the host response to many viral and bacterial infections by maximizing the kill efficacy of NK cells, macrophages and cytotoxic CD-8⁺ T-cells. However, abnormally high level of IL-18 was shown to correlate well with the severity of autoimmune and inflammatory diseases, such as Rheumatoid Arthritis (RA). Therefore, inhibition of IL-18 appears to be a valuable approach for treatment of inflammatory diseases. We have recently determined the high-resolution crystal structure of human IL-18 in complex with an inhibitory protein IL-18BP. From the structure, we obtained important atomic information as to the location of hot spots on IL-18 where potential small molecule inhibitors could be developed to block its bioactivity. We therefore carried out virtual screening and have identified a few potentially effective inhibitors of IL-18 signaling. Our competitive Elisa assay showed sub-micromolar Ki for these compounds and our preliminary data from cell-based assay indicated their effective inhibition on IFN-gamma production induced by IL-18. These compounds could serve as promising leads for further development of small molecule drugs for treatment of autoimmune and inflammatory diseases including RA.
10:20 AM - 11:40 AM Ballroom A
S4: Nanotechnology - Single-Walled Carbon Nanotubes

Chair: Donna Nelson (Chemistry & Biochemistry, The University of Oklahoma)
Presider: Christopher Brammer (Chemistry & Biochemistry, The University of Oklahoma)

10:20 T40 Effects of NaHCO₃ Washing and Change in Reagent Order upon the Reaction of Single-Walled Carbon Nanotubes with Thionyl Chloride and PMMA
Presenter: Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma
Authors and Affiliation: Donna J. Nelson, Christopher N. Brammer, and Murali Murugesan; Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK 73019, USA djnelson@ou.edu

Effects of sodium bicarbonate (NaHCO₃) washing upon Raman absorbances and electrical conductivities of single-walled carbon nanotubes (SWCNTs), before and after treatment with thionyl chloride (SOCl₂) and poly(methyl methacrylate) (PMMA), are explored. Increased Raman G/D ratios and reduced conductivities evidence that NaHCO₃ generally purifies SWCNTs. Upon treatment with SOCl₂, both p-SWCNTs and PMMA-wrapped SWCNTs have lower G/D ratios and increased conductivities, indicating SWCNT functionalization. Changing the ordering of SOCl₂ treatment and PMMA wrapping produces different products, which have different Raman spectra and electrical conductivities, and which are also influenced by NaHCO₃ washing.

10:40 T41 Horizontally Aligned Single Walled Carbon Nanotubes (SWNTs): Effect of H₂O on Defect Density and Film Uniformity
Presenter: Wesley Tennyson, School of Chemical, Biological & Materials Engineering, The University of Oklahoma

Realizing the full potential of SWNTs in electronics, optoelectronics, and sensors requires control of the alignment and position at the nanoscale. Directed growth to produce horizontally aligned carbon nanotubes has recently been demonstrated by numerous groups. We have investigated the growth of SWNTs with Fe as the catalyst, ethanol as the carbon source, and with varying concentrations of H₂O. We observed increased film density, reduced defect density, and a shift of the SWNT tube diameter distribution with changing in H₂O concentration. Additionally H₂O can halt the growth of SWNTs at higher concentrations.

11:00 T42 Controlled Functionalization of Single-walled Carbon Nanotubes with TEMPO-ended Polystyrene
Presenter: Abhijit Paul, Chemistry, Oklahoma State University
Authors and Affiliation: Abhijit Paul Warren T. Ford (Adviser) Department of Chemistry Oklahoma State University Stillwater, OK 74078

Single-walled carbon nanotubes (SWNTs) were functionalized with TEMPO ended polystyrene with different molecular weight using a “grafting to” technique. The TEMPO (2,2,6,6-tetramethyl-1-piperidinyloxy) ended polystyrenes (PS) of molecular weight 2000, 15,000 and 50,000 g/mol having polydispersity index (PDI) ranging from 1.13-1.36 were heated with mildly oxidized HiPCo SWNTs dispersed in 1-Methyl-2-pyrrolidinone at 130 °C. The amount of grafted polystyrene was determined by TGA analysis to be in the range of 25-30% by weight in all samples. In Raman spectra, there is little change in the intensity ratio (I_D/I_G) of D to G bands in any SWNT-PS grafted sample, which indicates that the functionalization of polystyrene did not change the inherent electronic properties of the SWNTs. This approach is promising in preparing SWNT based composite materials that retain the electronic properties of the SWNT.
T43: Synthesis of Functionally Graded Nanocoatings Using Initiated Chemical Vapor Deposition (iCVD)

Presenter: Yumin Ye, Biosystems Engineering, Oklahoma State University

Authors and Affiliation: Yumin Ye, Qing Song, Yu Mao Department of Biosystems Engineering Oklahoma State University

Synthesis of functionally graded coatings enhances the coating adhesion to substrates while maintaining the desired surface functionalities. We report an innovative method of creating functionally graded nanocoatings using a single-step initiated chemical vapor deposition (iCVD). By simply adjusting the flow ratio of the iCVD precursors at different deposition stages, the composition of the coatings can be altered at different depth in situ, resulting in different chemical functionalities across the entire thickness of the nanocoatings. We demonstrated synthesis of graded pH-responsive hydrogel nanocoatings directly on vertically aligned carbon nanotubes. The nanocoatings have an ultrathin crosslinked bottom layer above which the structure gradually changes to a pH-responsive hydrogel. The bottom layer has strong adhesion to the nanotube sidewalls, while the hydrogel layer changes the surface property of aligned nanotubes from hydrophobic (CA>112°) to superhydrophilic (CA< 5°). The hydrogel nanocoatings show thickness expansion of more than 30% by responding to pH change of 1. We also demonstrated one-step synthesis of graded antibacterial nanocoatings on a wide variety of materials. The nanocoatings are conformal, surface-adhesive and durable after repeated washing. In addition, the nanocoatings kill bacteria quickly (~100% bacteria reduction) by disrupting the cell membrane without leaching from the surface. Characterization results of the graded nanocoatings, including SEM, FTIR, AFM, etc., will also be presented.
2:00 PM - 5:10 PM Ballroom B
S7: Analytical and Physical Chemistry
Chair and Presider: Ivan Yip (Chemistry & Biochemistry, The University of Oklahoma)

2:00 T44 Electron Transfer Assisted Intersystem Crossing in Cyanoaromatics
Presenters: Paritosh Das, Physical Sciences, Cameron University
Authors and Affiliation: P. K. Das, Physical Sciences Department, Cameron University, Lawton, OK 73505.

Phenols and methylated/methoxylated benzenes efficiently quench the fluorescence of cyanoaromatics, e.g., 1,4-dicyanobiphenyl (DCB) and 9,10-dicyanoanthracene (DCA) with rate constants in the limit of diffusion control. Employing nanosecond laser flash photolysis, we have quantitatively measured the quantum efficiency of free-ion separation and triplet formation in the course of the charge-transfer quenching of DCN singlet excited state by a large number of phenols and methyl/methoxy benzene derivatives in acetonitrile. This paper will discuss the results in the light of free energy change for photo-induced electron transfer processes.

T45: Controlling the Amount of Dye Loaded on a Nanoparticle Surface
Presenter: Ronald Halterman, Chemistry/Biochemistry, University of Oklahoma
Authors and Affiliation: Kalani Gunawardana, Ronald L. Halterman, Department of Chemistry and Biochemistry, Lloyd A. Bumm, Department of Physics and Astronomy, University of Oklahoma, Norman

Modification of metal nanoparticle surface with organic dyes has been a subject of immense interest in recent years due to the novel application of such hybrid materials. To optimize the optical properties of these dye capped nanoparticles it is essential to control the loading density of dye on the nanoparticle surface. In this study we have introduced a simple method to control the loading of dye on gold nanoparticle surface using a competing ligand. We have loaded a BODIPY dye modified with alkenethioacetate tethers on citrate capped 16nm diameter gold nanoparticles in presence of a competing ligand, 11-mercaptooundecanoic acid. Under basic conditions, fluorescence measurements of sol/dye mixtures show that the loading of dye can be controlled by keeping the concentration of dye constant and varying the ligand concentration. Furthermore, using this data we have calculated the molar fluorescence of adsorbed dye on gold nanoparticle surface. The results show that the molar fluorescence of adsorbed dye decreases as the density of loaded dye increases.

T46: Quantification of Total $\omega$-6, Total $\omega$-3 and $\omega$-6/$\omega$-3 Ratio and Validation of Purdie Assay using GC-MS
Presenter: Mary Kimani, Chemistry, Oklahoma State University
Authors and Affiliation: Mary W. Kimani*, Gerard G. Dumancas, Neil Purdie, Lisa Reilly

Mary W. Kimani and Gerard G. Dumancas are Graduate Students and Neil Purdie is a Regents Service Professor, Department of Chemistry, Oklahoma State University, 018 Physical Science Building, Stillwater, OK 74078, USA; Lisa Reilly is an Assistant Professor at the Chemistry at Bethany College, Bethany, WV 26032, USA.

Qualitative determination of polyunsaturated fatty acids (PUFAs) in human serum has been of great challenge to researchers today. The work in this study has simultaneously quantified six PUF methyl esters, three that are the ($\omega$-6) esters of linoleic (LAME), conjugated linoleic (CLAME) and arachidonic (AAME) and three others that are ($\omega$-3) esters of linoleic (LNAME), eicosapentaenoic (EPAME), and docosahexaenoic (DHAME) fatty acids. Also calculated were the appropriate ($\omega$-6/$\omega$-3) ratios. These results and the results for serum cholesterol were also determined in the same assay in a time that is less than 40 minutes/sample, were validated against results measured using the gold standard GC/MS procedure. Blood serum aliquots taken from the same subjects were analyzed on the same day.
using GC/MS and visible spectrophotometric detections. Data obtained from GC/MS were quantified according to protocol. Spectral absorbance data from 350-550nm were analyzed using several chemometric models, the best of which was found to be PLS2. Results obtained from the two methods were correlated using student t-test and resulted in good agreements between total (ω-3) and total (ω-6) PUFA levels and for the (ω-6)/(ω-3) ratios. The significant accomplishment of the study was our ability to convert the mg/dL units from the spectroscopic method into percentages. This route was taken because the reverse is not possible to values to percentages which cannot be altered even when the integrated peak areas or peak heights obtained from GC/MS spectra are altered and has successfully validated Purdie assay.

T47: Pd Nanoclusters on Pristine and Functionalized Single-wall Carbon Nanotube: DFT and Experimental Studies

**Presenter:** Teerawit Prasomsri, Chemical Engineering, University of Oklahoma

**Authors and Affiliation:** Teerawit Prasomsri, Dachuan Shi, and Daniel E. Resasco

The carbon nanotube – inorganic oxide support decorated with Pd nanoclusters hybrid particles have recently shown a promising application in bio-oil catalyzed upgrading. These nanoparticles are capable to create the reactive solid-stabilized emulsion which can handle both aqueous and organic phases presented in bio-oils at the same time. The deposition and dispersion of Pd nanoclusters can be enhanced by creating defect sites on SWNTs which leads to a better metal - support interaction. The ONIOM(DFT:MM) was successfully applied for calculation of Pd nanocluster adsorption on SWNTs. The difference binding energies were investigated between the pristine and oxygen functionalized SWNTs. The calculation suggests that oxygen atoms at the defect sites can modify the electronic structure of SWNTs which results in a stronger bonding with the Pd nanoclusters. The experimental confirmation was conducted by the sputter coating technique. The result agrees well with the calculation, which shows more Pd nanoclusters anchored on the functionalized SWNTs, as compared to the pristine one.

T48: Silver-Alkenethiol Interaction Monitored from Plasmon Resonance

**Presenter:** Rama Krishna Ede, Department Of Mechanical And Aerospace Engineering, Oklahoma State University

**Authors and Affiliation:** Rama Krishna Ede and A. Kaan Kalkan, Functional Nanomaterials Laboratory, School of Mechanical and Aerospace Engineering, Oklahoma State University, Stillwater, OK 74078

The nature of the sulfur-metal bonding in self-assembly of alkenethiols on Au and Ag surfaces is not well understood. In particular, there is continuing debate, whether the metal behaves effectively as electron receiver or donor. The present work employs localized surface plasmon resonance (LSPR) associated with monolayers of Ag nanoparticles to quantify the chemisorption-induced electron transfer between silver and alkenethiols (vapor phase). The nanoparticles report the width (damping factor), intensity, and wavelength of the LSPR through optical extinction. These three parameters are plugged in a theoretical relation derived from Mie scattering to quantify the number of free electrons gained or lost (by the plasmon) due to the adsorbates. Hence, the chemisorption kinetics can be monitored from time-series optical extinction spectra. Our findings indicate bonding of alkenethiols to Ag is associated with electron transfer to Ag. Further, the kinetics of damping factor implies self-assembly. Therefore, LSPR spectroscopy is a promising alternative for elucidating the metal-alkenethiol interaction during self-assembly.

T49: Carbon Dioxide Generated In Situ by Carbamate for EOR Application

**Presenter:** Tzu-Ping Hsu, Petroleum Engineering, The University of Oklahoma

**Authors and Affiliation:** Ben Shiau, Tzu-Ping Hsu, Bruce Robert, Jeffrey H Harwell

Carbon dioxide injection to reservoir has been widely investigated for enhanced oil recovery application. The beneficial effects of CO2 are well known, which include increasing the reservoir rock permeability for oil and decreasing the oil viscosity. Recently, a physicochemical enhanced oil recovery (EOR) method which generates CO2 in situ has been studied in the oil fields by few researches in Russia. It has been reported that the use of carbamate in surfactant-based system, generating CO2 and alkaline buffer solution in situ. Due to the heat energy of the formation or that of the injected heat carrier, carbamate is subjected to hydrolysis to yield CO2 and ammonia. However, limited references in this area are available. To explore this idea, our research group has been working on the feasibility study of carbamate for generating CO2 in situ in EOR application. In our preliminary study, several chemicals were investigated for their potential to engender CO2 under high temperatures. Results showed that at temperature greater than 85°C, ammonium carbamate can produce carbon dioxide. In contrast, no CO2 evolved was observed while heating up the methyl carbamate. Ammonium carbamate was further studied in one-dimensional column. At temperature higher than 858°C, ammonium carbamate produced CO2 in the columns, changing oil property by decreasing oil viscosity. For example, an additional injection of 0.5 PV of 3% ammonium carbamate solution to a chemical flood process (polymer + surfactant) improved 9.7% (OOIP) of crude oil recovery. Instead of looking black, the crude oil coming out from the carbamate injected column looked dark brown and less viscous. This may imply that the property of crude oil was changed by the CO2 generated in the column. The experiment also found that AMP (2-Amino-2-methyl-1-
propanol) which is normally used for carbonate dioxide capture in power plant was also a promising candidate for generating carbon dioxide under high temperatures. Currently, our research group continues studying different potential carbamates that can produce CO₂ under high temperatures. We are also trying to introduce carbamates to the surfactant systems developed by our lab for EOR application. Carbon dioxide generated by carbamate in surfactant system is anticipated to decrease the oil viscosity while dissolved in the oil and/or increase the viscosity of surfactant system by creating foam. In addition, the oils with different viscosities, such as decane and light crude oil, are being tested using one-dimensional column to investigate the main mechanisms improving oil recovery by carbamates. In future work, core flood study will be conducted to simulate the reservoir conditions.

T50: Micelle Simulations with GB Implicit-Solvent Models: Parameterization and Application to pKa Predictions of Surfactants in Micelles
Presenter: Yuhang Wang, Chemistry and Biochemistry, University of Oklahoma
Authors and Affiliation: Yuhang Wang, Jason A. Wallace and Jana K. Shen Department of Chemistry and Biochemistry University of Oklahoma

The surfactant micelle systems, especially its hydrophobic and dielectric properties, have been studied for a long time. But the micro-scale interactions are still not well understood. The pKa shift, as a result of the electrostatic interactions as well as other factors, is a good indicator of the special characters of the micelle surface micro-environment. Here, the pKa shift behavior of a single lauric acid(LAU) in the surfactant micelle was studied using constant-pH-molecular-dynamics coupled with the replica-exchange method. Three different types of surfactant micelle systems were chosen: sodium dodecyl sulfate(SDS), dodecyl trimethyl ammonium chloride(DTA) and dodecyl triethylene glycol ether(DE3). The resulting pKa's of LAU from the simulation match the experimental results well for SDS and DE3 micelle, while limitations were found for DTA micelle due to several assumptions made in the technique. Radial distribution function calculation shows that the relative distance between like- and dislike-charges are important for the titration. These results indicate that simple polar and nonpolar interactions are not sufficient for the description of the surfactant micelle surface and the dielectric interface effects are key to the pKa shift of the protonation reaction on the surface.

T51: Vibrational Spectroscopic and X-Ray Crystallographic Study of Secondary Amine/Phosphoric Acid Systems
Presenter: Dharshani Bopege, Physics & Astronomy, University of Oklahoma
Authors and Affiliation: Dharshani N. Bopege (a),*, Roger Frech (b), D.T Glatzhofer (b), D. Powell (b) (a) Department of Physics and Astronomy, The University of Oklahoma, Norman, OK, 73019 (b) Department of Chemistry and Biochemistry, The University of Oklahoma, Norman, OK, 73019

Linear and branched poly (ethyleneimine) (PEI)-acid systems have been widely studied during past few years because of their potential as polymeric proton conductors. It has been shown that the membranes made from these materials exhibit good proton conducting properties. As a consequence, these materials are candidates as electrolytes for constructing H₂/air fuel cells. However, because of complex structures of polymer electrolytes, model compounds are needed to explain the local structure of polymer electrolytes.

The aim of the present work is to understand the hydrogen bonding network of secondary amine - phosphoric acid model compounds. Particularly, protonation of nitrogen atoms in the backbone of the amine leads to hydrogen bonding which is observed in the NH stretching mode and the NH bending mode. These modes can be generally recognized using Fourier Transform Infrared and Raman spectroscopy.

In the present work, we studied diethylene amine and N,N’-dimethylethylenediamine complexed with phosphoric acid. We prepared two crystals; their structures were solved by X-ray diffraction methods. Examined vibrational spectra of both crystals revealed distinct broad IR bands at 2300-2600 cm⁻¹ for the NH₃⁺ stretching mode and bands at 1500-1700 cm⁻¹ for the NH₃⁺ bending mode. This clearly agrees with literature values for PEI-acid systems.
2:00 PM - 3:30 PM Ballroom G
S8: Biochemistry
Chair and Presider: Paul Sims (Chemistry & Biochemistry, The University of Oklahoma)

2:00 T52 The Neuraminidase Activity of Human Parainfluenza Viruses 1, 2, and 3
Presenter: Mary Tappert, Biochemistry and Molecular Biology, University of Oklahoma Health Sciences Center
Authors and Affiliation: Mary Tappert, Shelly Gulati, and Gillian Air; Department of Biochemistry and Molecular Biology; University of Oklahoma Health Sciences Center Oklahoma City, OK 73104

The human parainfluenza viruses (hPIVs) are the second-leading cause of respiratory tract disease in children. Their hemagglutinin-neuraminidase surface glycoprotein has both hemagglutinin (H) activity (the ability to agglutinate red blood cells, thought to correspond to receptor-binding function) and neuraminidase (N) activity (the ability to release sialic acid from substrates, thought to correspond to receptor-destroying function). HN is the major antigen of hPIVs and is therefore a prime target for drug therapies and vaccines. Despite HN’s potential biological and therapeutic importance, however, its role in infection remains unclear: does it truly both recognize and destroy receptors? Does one activity predominate? We analyzed the enzyme activity of N using a variety of substrates: the small molecules 2′-(4-methylumbelliferyl)-N-acetylneuraminic acid (MUN) and 3′N-acetylneuraminylactose (3′NANL), the glycoproteins bovine fetuin and human α1-acid glycoprotein (AGP), and a proteinase K digest of fetuin (fetuin peptides).

hPIV1 and 2 Ns cleave all five tested substrates. Although they exhibit similar affinity (Km ≈ 0.5-1 mM) for all five, their cleavage activity (Vmax) is 5-10-fold higher on MUN and 3′NANL than on glycoproteins or glycopeptides. hPIV3 N cleaves MUN and AGP but not 3′NANL, fetuin, or fetuin peptides; its affinity and activity are weaker than hPIV1 and 2 on MUN (Km ≈ 10 mM and Vmax ~ 2-fold lower) but in the same range as hPIV1 and 2 on AGP. At pH 5, hPIV2 and 3 cleave receptors on red blood cells, while hPIV1 does not. The data so far indicate that the N of hPIV2 and 3 cleave their receptors, while some hPIV1 receptors are resistant. Interestingly, receptor-destroying function appears to be independent of total neuraminidase activity as measured in solution assays.

T53: Functional Role of Active Site Residues, Glu78, Glu122, H96 and Lys99 of Saccharopine dehydrogenase from Saccharomyces cerevisiae
Presenter: Devi Ekanayake, Department of Chemistry and Biochemistry, University of Oklahoma
Authors and Affiliation: Devi Ekanayake, Kostyantyn Bobyk, Babak Andi, Ann H. West, Paul. F. Cook.

Saccharopine dehydrogenase catalyses the NAD+-dependent oxidative deamination of saccharopine to give L-lysine and α-ketoglutarate. Data obtained previously and a semi-empirical model of the E-NAD-saccharopine ternary complex suggested Glu78, Glu122 Lys97 and/or His96 as potential catalytic group to accept a proton from the secondary amine of saccharopine in the hydride transfer step and/or to activate a water molecule in the imine hydrolysis step. There are many ionizable groups in the active site suggesting that they all are important for the overall SDH reaction. Site directed mutagenesis was used to generate E78A, E122A, H96Q, K77M, D319A, K99M and E78A/E122A mutant enzymes. The kinetic mechanism remains the same as that of wild type for all the mutant enzymes. Largest change observed for V was 100- fold change for H96Q indicating that it plays a catalytic role. Isotope effects suggested K77M also important for catalysis as well. Large changes in V/KLys, for E78, K99M and E122 suggest that contribute binding energy for lysine. Substrate, solvent and multiple isotope effects are in agreement with the kinetic data and the overall chemical mechanism. The pH-rate profiles exhibit shifts in the pKα values to higher and lower pH, which suggests the presence of E78, and E122 modulates the basicity of the catalytic groups. Results are discussed in terms of proposed chemical mechanism.
α-Aminoadipate pathway for lysine biosynthesis is nearly unique to higher fungi, including human and plant pathogens and euglenoids. An exception is the thermophilic bacterium *Thermus thermophilus*. Homocitrate synthase (HCS) catalyzes the first and regulated step of the pathway, condensation of acetyl-CoA and α-ketoglutarate to give homocitrate and CoA, and as a result it is a potential target for the development of new antifungals against Candida albicans, Aspergillus fumigatus and others. Saccharomyces cerevisiae HCS and Candida albicans HCS are extremely unstable, and thus limit biochemical and structural studies. As a result, the kinetic and chemical mechanism of the HCS from *Thermus thermophilus* is being characterized. The Saccharomyces cerevisiae HCS is a Zn-metalloenzyme, while the one from *Thermus thermophilus* is inhibited by Zn$^{2+}$ and requires Mn$^{2+}$ or Mg$^{2+}$ for activity. The kinetic mechanism of THCS is ordered with α-ketoglutarate (αKg) adding prior to acetyl CoA (AcCoA), but with Mg$^{2+}$ is steady state random with a preferred order the same as with Mn$^{2+}$. The deuterium isotope effect measured with acetyl-d$_3$ CoA is unity at low AcCoA being measured. Data are discussed in terms of the mechanism of HCS and are compared to that obtained for the yeast enzyme.

This work was supported in part by funds from the Grayce B. Kerr endowment to the University of Oklahoma to support the research of P.F.C.
Methyl esters can be derived from various renewable sources such as vegetable oils and biomass. This study will focus on several aspects of conversion of methyl esters over supported platinum catalysts including reaction mechanisms, catalyst design, and production of targeted products. Methyl octanoate and methyl hexanoate are used as probe molecules. Catalysts are characterized by CO chemisorption, TPR, TPO, and XPS techniques. In the gas-phase reaction of methyl octanoate in hydrogen, 1%Pt/Al2O3 is an active and selective catalyst. The dominant products are C7 hydrocarbons, which come from deoxygenation reactions of various ester-derived oxygenates. When titania replaces alumina, hydrogenation reaction of the ester is promoted, leading to an increase in C8 hydrocarbon selectivity. Without hydrogen, 1% Pt/Al2O3 catalyst deactivates quickly owing to coking.

This prompts us to further study the behaviors of different platinum catalysts in conversion of an ester without hydrogen. In the gas-phase reaction of methyl hexanoate over silica-supported Pt-Sn-K catalysts, it was found that coupling or condensation products (i.e. ketonization products) are formed first. Subsequently, these are transformed into lighter oxygenate compounds and hydrocarbons (mainly C5 and C6) via decarboxylation and decarbonylation routes. Silica support itself shows a low level of conversion of methyl hexanoate in helium. All of its activity goes to formation of condensation products. These condensation products, together with surface carboxylates and ester molecules, oligomerize to form “oxygenate” type of coke on silica. 1% Pt/SiO2 is active at the beginning of methyl hexanoate reaction due to clean Pt ensembles available. However, pure platinum catalyst deactivates quickly to form “aromatic” type of coke. This carbonaceous species supply a source of hydrogen via dehydrogenation reactions. It is the spilled-over hydrogen that cleans the silica support for condensation reaction after Pt/SiO2 deactivates. Additions of Sn and K into platinum have several simultaneous effects. Firstly, the Pt ensembles are ruptured owing to Sn and K coverage and formation of Pt-Sn alloy. Secondly, potassium enhances the segregation of Sn out of Pt-Sn alloy. The addition of appropriate amount of Sn into Pt shows a positive impact on the conversion of methyl hexanoate. Adsorption energy of the ester is reduced on Pt-Sn alloy due to the facilitated interaction of the ester molecule with cationic Sn species. It is the alloy that extends the lifetime of Pt-Sn catalyst by promoting desorption of alkene-derived coke precursors. As a sequence, coke deposit is reduced on 1%Pt-1.3%Sn/SiO2 catalyst compared to pure platinum catalyst. The introduction of a third metal, potassium, enhances the overall activity even further. Potassium domains accompanied by SnO2 are effective in converting the original ester into coupling products, which are then transformed into hydrocarbons on the available Pt ensembles of Pt-Sn-K catalysts. Among all tested Pt-Sn-K catalysts, 1%Pt-1.3%Sn-0.5%K/SiO2 exhibits the highest activity and stability in reaction of methyl hexanoate under helium.

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T59: Vanadyl meso-Tetraphenylporphyrin Catalyzed Pinacol Coupling Reactions in Water

**Presenter:** Ronald Halterman, Chemistry/Biochemistry, University of Oklahoma

**Authors and Affiliation:** Shekar Mekala, Jessica P. Porterfield, Ronald L. Halterman, Department of Chemistry and Biochemistry, University of Oklahoma, Norman

The pinacol coupling reaction of aldehydes to form vicinal diols is developing into a versatile method for carbon–carbon bond formation, which could be very useful in conversion of biomass-derived oxygenated feedstocks into value-added chemicals and biofuels. Several low-valent metals have been employed in stoichiometric amounts to reduce aldehydes to ketyl radicals that can then dimerize to form meso- or dl-isomers of 1,2-diol products. Recently, we have investigated the pinacol coupling of benzaldehyde (0.25 M or 1.25 M) in water catalyzed by 5 mol % CrCl2 in the presence of Zn-dust or Al-dust at 20 °C or 60 °C. In all cases, the pinacol coupling product, 1,2-diphenyl-1,2-ethanediol, was obtained along with benzyl alcohol, being formed by a competitive 2e− reduction of the carbonyl. Now, we are investigating the pinacol coupling of other aldehydes such as furfural and cyclohexanecarboxaldehyde in water catalyzed by Vanadyl meso-tetraphenylporphyrin in presence of Al-dust or Zn-dust or Mn at 60 °C.

T60: Nanohybrid Particles that Catalyze Biofuel Upgrade Reactions at the Interface of Water/Oil Emulsions

**Presenter:** Jimmy Faria, Chemical, Biological and Materials Engineering, University of Oklahoma

**Authors and Affiliation:** Jimmy Faria, Santiago Drexler, Paula Zapata, Min Shen, Daniel E. Resasco* University of Oklahoma. Department of Chemical, Biological, and Materials Engineering

The pyrolysis of biomass is one of the most technically and economically feasible processes for the production of alternative fuels. The pyrolysis process converts solid biomass into gases, char, and liquid (Bio-oil). The latter is an unstable biphasic mixture of oxygenated molecules (furfurals, guaiacols, phenols, small acids and aldehydes) with water. In this context, a very convenient strategy for the refining of bio-oil could be the utilization of a recoverable and recyclable solid catalyst that naturally segregates to the water-oil interface. Therefore, the main objective of this project is to perform catalytic upgrading reactions (condensation and hydrodeoxygenation) at the water-oil interface of emulsions, using transition metals (Pd) supported on solid nanohybrid particles based on carbon nanotubes fused to metal-oxides (SiO2 and MgO).

T61: Model Compound Study of Phenolic Compounds Conversion over Acidic Zeolites During Bio-Oil Up Grading

**Presenter:** Xinli Zhu, School of Chemical Biological And Materials Engineering, the University of Oklahoma

**Authors and Affiliation:** Center for Biomass Refining, School of Chemical, Biological, and Materials Engineering, The University of Oklahoma, Norman, OK 73019, USA

Phenolics compounds are a family of compounds derived from lignin biomass via fast pyrolysis (and/or liquefaction and/or solvolysis). The major functional groups of phenolics are hydroxy group (–OH) and methoxy group (–OCH3). Methoxybenzene (anisole) was selected as a model compound to represent the –OCH3 group of phenolic compounds conversion during bio-upgrading over acidic zeolites. Conversion of anisole was studied over an HZSM-5 zeolite at varying space times (W/F), reaction temperatures, type of carrier gas, and concentration of water in the feed. Several bimolecular and unimolecular reactions are proposed to take place. The bimolecular reactions include the following transalkylation reactions: a) anisoles to phenol and methylanisole; b) phenol and methylanisole to cresols; c) phenol and anisole to cresol and phenol; d) methylanisole and cresol to phenol and xylol. A pseudo first-order kinetic model based on these bimolecular reactions was found to describe well the observed product distribution as a function of W/F. Shape selectivity effects prevail over electrophilic substitution and thermodynamic equilibrium effects in the formation of methylanisole isomers. However, the opposite is true for the distribution of cresol isomers. The kinetic analysis indicates that the contribution of unimolecular reactions such as isomerization is much lower than that of bimolecular reactions. When H2 was used as a carrier, catalyst stability showed slightly improvement in comparison to the runs under He. Remarkably, addition of water was found to increase catalytic activity significantly.
SWNT-silica-polystyrene composites can be successfully synthesized via a Pickering miniemulsion polymerization method. Styrene-in-water emulsions were first generated by SWNT-silica hybrids heavily oxidized by HNO3, then in-situ polymerization was carried out to form sphere polystyrene particles covered by SWNT-silica hybrids. This core-shell structure was confirmed by a combination of techniques including SEM, TEM, AFM, XPS and elemental mapping. The effects from water/monomer volume ratio, amounts of initiator, and particle concentration on particle structure and polymerization rate were investigated. The conductivity measurements on these materials suggest a better dispersion of the SWNTs compared with simply mixing by dissolving. Finally, the same protocol was followed to successfully synthesize MWNT-Al2O3-polystyrene sphere particles. This indicates that this surfactant-free polymerization technique can be a general strategy for making polymer sphere particles coated by carbon nanotubes.

T63: Interfacially Active SWNT/Silica Nanohybrid Used In Enhanced Oil Recovery
Presenter: Luis Villamizar, Petroleum Engineering, University of Oklahoma
Authors and Affiliation: Luis Villamizar, Prapas Lohateeraparp, Jeffrey Harwell, Daniel Resasco, Ben Shiau; Chemical Science and Material Science – Petroleum Engineering; The University of Oklahoma

Single-Walled-Carbon-Nanotube (SWNT)-Silica nanohybrid particles are a very promising material for enhanced oil recovery because of their interfacial activity. The mechanism used to recover additional oil would be to deliver catalytically active nanohybrid particles to the O/W interface, where they would react and modify the oil properties to mobilize the oil in the reservoir. In order to do that the particles were dispersed in an aqueous solution by using polymer and after that one-dimensional-sand-pack studies were performed to evaluate the flow of the nanohybrid particles through porous media. The results showed that the most of the nanohybrid particles not only could pass through but also about half of the particles injected will go the O/W interface when the porous medium contains a residual saturation of hydrocarbon, where they could be used to support a catalytic conversion of components of the oil.

T64: Counter-Flow Diffusion Flame Synthesis of Polygonal and Ribbons-Like Tungsten Oxide Nanostructures
Presenter: Wilson Merchán-Merchan, Aerospace and Mechanical Engineering, The University of Oklahoma
Authors and Affiliation: Wilson Merchán-Merchan, Alexei V. Saveliev2, and Walmy Cuello Jimenez1
1School of Aerospace and Mechanical Engineering, University of Oklahoma, Norman, OK 73019, USA
2Department of Mechanical & Aerospace Engineering, North Carolina State University, Raleigh, NC 27695, USA

1-D and 3-D tungsten-oxide nanostructures were formed on high purity tungsten wires introduced in a counter-flow diffusion flame. The influence of the oxygen content and probe diameter on the growth of tungsten-oxide nanostructures was studied in order to gain more insight in the formation mechanism of these novel structures. The synthesis of 1-D nanorods on the upper surface of the tungsten wire probe was observed when 1 mm diameter wires were inserted into the flame medium with an oxidizer composition of 50%O2 + 50%N2. 3-D polygonal-shape structures such as triangular, rectangular, square, and cylindrical channels with completely hollow or semi-hollow morphology were obtained by decreasing the probe diameter to 0.5 mm. Conversely, the increment of the O2 content to 100% along with the employment of 1 mm diameter probes resulted in the formation of ribbon-like micron-scaled structures. High-resolution TEM analysis showed that the synthesized structures have a lattice spacing of ~0.38 nm which closely resembles a monoclinic WO3 structure. X-ray photoelectron spectroscopy analysis revealed that the larger 3-D structures are also made of WO3 corroborating that the chemical composition of the structures remains the same whilst varying the probe and flame parameters. The proposed growth mechanism states that the 3-D WO3 structures are formed through the lateral coalescence of 1-D W oxide nanorods.
T65: Novel Nanovectors for Targeted SKBR-3 Breast Cancer Cell Imaging and Destruction

Presenter: Gopal Abbineni, Chemistry & Biochemistry, University of Oklahoma

Authors and Affiliation: Gopal Abbineni and Chuanbin Mao University of Oklahoma, Chemistry and Biochemistry Department, Norman, OK-73019.

The objective of this work is first, to identify epithelial breast cancer cell specific ligands using phage display technology and second, to isolate the target specific peptide from selected phage and third to conjugate the isolated protein on the surface of the functionalized gold nanorod to synthesize phage like nanoparticles (PLN’s) and observe its applications in breast cancer cell imaging and destruction. The synthesized PLN’s can selectively bind to the surface of a breast cancer cell through receptor-ligand interactions and can selectively destroy the cancer cell when exposed to Near Infrared radiations (NIR). These conclusions are based on the following observations. First, phage library can be used to identify peptides that can specifically target a desired cell. Second, Goldnanorods (AuNRs) exhibits surface plasmon resonance and hence can absorb NIR and convert Light into heat. Third, Gold nanorod exhibits scattering properties and fourth, isolated proteins can be easily conjugated onto functionalized AuNRs. Our results to date show that these PLN’s can improve the ability of AuNRs to detect the cancer cells more efficiently than the conventional probes and can selectively kill the cancer cells upon NIR irradiations. Thus these PLN’s can serve as a next generation nanovectors for imaging and destruction of breast cancers. We are currently investigating the mechanism of entry of these nanovectors into the targeted SKBR-3 breast cancer cells.
2:00 PM - 6:00 PM Ballroom C

S9: Organic Chemistry

Chair and Presider: Donna Nelson (Chemistry & Biochemistry, The University of Oklahoma)

2:00 T66 Hollywood Chemistry

2:20 T67 Effects of Ligand Structure and Donor Type on Catalytic Activities of Electrophilic (Chelate)Palladium(2+) Complexes

2:40 T68 Ligand-Accelerated Intramolecular Amination

3:00 T69 Synthesis of Metabolites of the Heteroarotinoid Drug SHetA2

T66: Hollywood Chemistry

Presenter: Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma

Authors and Affiliation: Donna J. Nelson* and Christopher N. Brammer, Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK 73019 djnelson@ou.edu

Connections between chemistry and Hollywood surround us. Albuquerque high school teacher Walter White (Bryan Cranston) teaches high school organic chemistry in the AMC television series "Breaking Bad." As another example, Academy Award Producer Gray Frederickson (Godfather Part 2) collaborates on Eminent Scientist filming in Oklahoma; the first subject we selected to film was organic chemistry Professor E. Ann Nalley. Examples of our growing scientific connections with Hollywood and the resulting influences will be discussed.

T67: Effects of Ligand Structure and Donor Type on Catalytic Activities of Electrophilic (Chelate) Palladium(2+) Complexes

Presenter: LeGrande Slaughter, Chemistry, Oklahoma State University

Authors and Affiliation: Sri S. Subramanium, Department of Chemistry, Oklahoma State University LeGrande M. Slaughter (corresponding, presenting), Department of Chemistry, Oklahoma State University

N-heterocyclic carbenes (NHCs) are strong donor ligands used in metal catalysis of many organic reactions. Bidentate bis(carbene) ligands offer potential stability advantages due to the chelate effect and could allow tuning metal reactivity through bite angle variation. A series of dicationic bis(carbene) and bis(phosphine) complexes of palladium(II) were prepared and studied to assess the effects of carbene structure and bite angle on effective donor ability. As such, it relates to electrophilic catalysis. Methylisocyanide adducts of various [(chelate)Pd]Cl2 fragments were examined by IR spectroscopy to determine a scale of relative trans influence, and hence effective donor strength, for bidentate ligands. Studied ligands included imidazole-derived bis(NHCs), bis(acyclic diaminocarbenes), bitriazole bis(NHCs), and "abnormal" C4-bound bis(NHCs). Structural studies allowed trends in effective donor ability to be correlated with structural parameters such as carbene dihedral angle. To test the predictive ability of these assessments, [(chelate)Pd]Cl2 complexes were examined as catalysts for the formation of cyclic alkenyl ethers from acetylenic aldehydes. The most active catalysts were those with ligands predicted to have low effective donicity by the MeNC IR probe studies. Thus, bis(carbene) ligands can be tuned to support electrophilic catalysis by metals, in contrast to the prevailing use of mono-NHCs to engender electron-rich metal centers.

T68: Ligand-Accelerated Intramolecular Amination

Presenter: Dipti Barman, Chemistry and Biochemistry, University Of Oklahoma

Authors and Affiliation: Mr. Dipti N. Barman, University Of Oklahoma; Dr. Kenneth M. Nicholas, University Of Oklahoma

The amino functional group is an important and widely used component in biology and medicinal chemistry. Its importance has recently inspired chemists to design a variety of amination methodologies involving C-H bond activation. Our group is seeking to develop new catalytic intramolecular amination reactions of carbamates and sulfamates to generate in-situ nitrenoid species, which are reacting by Cu-catalysts. The scope and selectivity of these reactions was investigated with a range of benzylic substrates.

T69: Synthesis of Metabolites of the Heteroarotinoid Drug SHetA2

Presenter: Baskar Nammalwar, Department of Chemistry, Oklahoma State University

Authors and Affiliation: Baskar Nammalwar, 1 Richard. A. Bunce,1 K. Darrell Berlin1 and Tao Lu1 1) Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma 74078; 2)College of Basic Sciences at the China Pharmaceutical University, Nanjing, China

A new route was developed for the synthesis of metabolites of SHetA2, which is currently in preclinical studies. The synthesis of these metabolites may increase the hydrophilicity of the target drug, which in turn might increase the potency of the compound. The synthesis required a 17-step route to achieve the target metabolites in an overall yield of 4.2%. The strategy involved several key reactions such as cyclization of a 2,2-dimethylthiochroman-4-one ring system, conversion of the 4-keto group to 4-methyl-4-hydroxymethyl substitution, nitration of aromatic ring, reduction to the aniline and reaction with p-nitrophenylisothiocyanate. The presentation will cover the steps involved in the synthesis and the challenges confronted in the formation of these metabolites. Preliminary modeling studies have revealed that the metabolite binds with a KIT kinase via H-bonding to Cys 673, Thr 670 and Glu 640. Further studies on these metabolites are currently underway and the initial results are promising.
3:50 PM - 6:00 PM Ballroom G

S10: Environmental Chemistry
Chair and Presider: Mark Nanny (School of Civil Engineering & Environmental Science, University of Oklahoma)

3:50 T70 Using Solid-State Deuterium NMR to Characterize the Association of Benzene with Humic and Fulvic Acids
Presenter: Mark Nanny, School of Civil Engineering & Environmental Science, University of Oklahoma
Authors and Affiliation: Margaret A. Eastman, Oklahoma State University, Chemistry, Stillwater, OK, 74078-0447; Lucinda C. Brothers, University of Oklahoma, Chemistry, Norman, OK, 73019-0631; Mark A. Nanny, University of Oklahoma, Civil Engineering and Environmental Science, Norman, OK, 73019-0631

Interactions of hydrophobic pollutant organic molecules with humic substances affect the fate of these molecules in the environment. We present the first application of solid-state 2H quadrupole-echo NMR techniques to obtain insight into the interactions of the aromatic hydrocarbon benzene-d6 with humic and fulvic acids. Sorbed benzene-d6 appears to undergo two types of motion, isotropic (ISO) and a restricted small-angle wobble (SAW) motion. SAW motion is most likely due to an adsorption-like interaction with more rigid regions of the humic acid, while ISO motion may be due to dissolution of the benzene in more flexible regions or tumbling within pores. A substantial increase in the percentage of SAW with aging over a period of many months implies that benzene-d6 slowly penetrates into the humic acid. For benzene undergoing SAW motion there are at least two and perhaps a series of T1 values, indicating more than one sorption environment.

T71: Individualization of Gasolines by GCIRMS Fingerprinting
Presenter: Tomasz Kuder, Geology, University of Oklahoma
Authors and Affiliation: Tomasz Kuder and Paul Philp
School of geology and Geophysiscs University of Oklahoma, Norman

Individualization of gasolines is of interest in arson cases (e.g., correlation between gasoline residues recovered from fire debris and from a suspect) and in environmental pollution cases (identification of potential contamination sources). GCMS fingerprinting utilizing multivariate statistics for data interpretation has been applied in such studies. Compound-specific isotope analysis (CSIA) of gasoline hydrocarbons provides another dimension for sample individualization. Isotope signatures of gasolines reflect variations in their petroleum precursors and the refining/reforming processes. As the result, the same chemical compounds produced at different facilities, or produced at different periods may have distinct isotope ratios.

This presentation demonstrates the potential of CSIA fingerprinting on aromatic hydrocarbons in a set of 37 commercial gasolines. A pair-wise fingerprint comparisons utilizing carbon, hydrogen and combined two-isotope fingerprints were performed. A combination of carbon and hydrogen data was most powerful, allowing differentiation of 46% of the tested gasoline pairs. The main benefit of the CSIA approach is relative simplicity of data interpretation. The CSIA approach does not involve a multivariate statistical analysis; the difference in isotope ratios is an objective criterion of sample difference. In general, CSIA data allowed higher degree of specimen individualization than GCMS fingerprints.
T72: Characterization of Naphthenic Acids in Petroleum Process Waste Water

**Presenter:** Mark Nanny, School of Civil Engineering & Environmental Science, University of Oklahoma

**Authors and Affiliation:** Aaron M. Westbrook, Chemical, Biological and Material Engineering, University of Oklahoma, Norman, OK 73019; Mark A. Nanny, Civil Engineering and Environmental Science, University of Oklahoma, Norman, OK, 73019

Naphthenic acids (NA) are often present in crude petroleum and comprise a complex mixture of alkyl-substituted acyclic and cycloaliphatic monocarboxylic acid compounds with an empirical formula of C\(n\)H\(2n+Z\)O\(_2\) where “n” and “Z” respectively represent the number of carbon atoms and cyclic structures. NA are corrosive to processing equipment and toxic to aquatic organisms, however their polarity and aqueous solubility, as well as low biodegradability, makes their removal from aqueous waste streams challenging. Naphthenic acids from three petroleum processing waste water samples were isolated using XAD-8 resin, derivitized with N-methyl-N-(tert-butylidemethylsilyl)trifluoroacetamide, characterized with gas chromatography-mass spectroscopy (GC/MS) and then analyzed in 3-D plots of peak area, n, and Z. Improvement of analytical method by using GC peak area for quantification of NA and aligning each NA compound to a single MS parent peak in 3-D plot ensures each NA compound has been represented only once on 3-D plot with accurate “n” and “Z” values. Each petroleum process waste water sample contained NA mixtures with n values ranging from 5-15 with Z values ranging from 0 to -2, indicating the presence of small carbon chained acyclic and monocyclic NA. Data suggesting the presence of dicarboxylic acids was tested with known standards.

T73: Enhancing Microbial Methanogenesis of Coal by Ozonolysis

**Presenter:** Mark Nanny, School of Civil Engineering & Environmental Science, University of Oklahoma

**Authors and Affiliation:** Mary Züñiga, School of Civil Engineering and Environmental Science, College of Engineering, University of Oklahoma, Norman, OK; Margarita Mendivelso, Department of Botany and Microbiology, College of Arts and Sciences, University of Oklahoma, Norman, OK, Institute for Energy and the Environment, College of Earth and Energy, University of Oklahoma, Norman, OK; Joseph M. Suflita, Department of Botany and Microbiology, College of Arts and Sciences, University of Oklahoma, Norman, OK; Institute for Energy and the Environment, College of Earth and Energy, University of Oklahoma, Norman, OK; Mark A. Nanny, School of Civil Engineering and Environmental Science, College of Engineering, University of Oklahoma, Norman, OK, Institute for Energy and the Environment, College of Earth and Energy, University of Oklahoma, Norman, OK

Six coals ranging in rank from lignite to bituminous with low to high volatile matter content were subjected to ozonolysis as aqueous slurries to test the hypothesis that ozonolysis as aqueous slurries to test the hypothesis that the reduced nature of coal organic carbon limited biogenic methanogenesis. Thus, mild oxidation of coal should enhance microbial methanogenesis relative to unozonated coal. An inoculum collected from production waters from a major coal formation was incubated with the various coals. A greater rate and extent of methanogenesis was observed for ozonated relative to unozonated particulate lignite. In contrast, few differences were observed with the other ozonated and untreated particulate coals. However, three of the inoculated aqueous effluents from the ozonation procedure produced methane at a rate that ranged from 3.1 to 7.9 μmoles/day and was at least five times the rate measured with the particulate coals. BET surface area and pore size distribution analysis showed only a small increase (approx. 10%) in coal particles upon ozonation. Infra-red (IR) spectroscopy of the coals demonstrated that ozonolysis did not significantly change the coal particle surface; presumably as the surface is oxidized, the reagents are sloughed off into solution, exposing a fresh coal surface. However IR spectroscopy showed that the aqueous effluent composition varied as a function of each coal, and consisted of compounds containing carboxylate, aldehyde, and ketone functional groups that are clearly more amenable to anaerobic decay and biogenic methanogenesis.

T74: Environmental, Synthetic, and Materials Applications of Tungsten Trioxide

**Presenter:** Hamed Albusaidi, Chemistry, OSU

**Authors and Affiliation:** Hamed Albusaidi, Dr. Apblett, A. W.

Uranium has widespread environmental concern due to its chemical toxicity and radioactivity. Despite the fact that little is known about the effects of long term uranium exposure in humans, the major health effect of uranium ingestion is kidney toxicity. Lead and cadmium are also toxic metals that target the soft tissues of the human body. A variety of methods have been used for removing uranium from ground water but unfortunately commonly used water treatment processes are not effective. We will report the results of an investigation of the effectiveness of tungsten trioxide and tungstic acid to remove uranium from drinking water. This technique was also used to remediate water contaminated with other toxic metals such as cadmium and lead. We will report the results of competition reactions between calcium and magnesium and the toxic metals for uptake by tungsten trioxide and tungstic acid. The success of the remediation process led us to develop a new synthetic methods for alkaline earth and transition metals tungstates.
T75: Green Chemistry Laboratory: Molybdate Processing of Copper Ore
Presenter: Kevin Barber, Chemistry, Oklahoma State University
Authors and Affiliation: Kevin N. Barber, Allen W. Apblett, Department of Chemistry, Oklahoma State University, Stillwater, OK

There is significant interest in alternative environmentally friendly processing of metal ore materials, especially those that alleviate the need for roasting of sulfide ores and can be carried out under mild thermal and chemical conditions. The purpose of this presentation is to illustrate a straightforward green chemistry laboratory aimed at an undergraduate audience. The student starts with a synthetic copper ore (malachite), performs an extraction step, a precipitation with a molybdate reagent, separation, simultaneous recovery of molybdate reagent for recycling and precipitation of copper hydroxide, and finally carbothermal reduction to copper metal. The student obtains an understanding of the chemical fundamentals of ore processing (extraction, reduction), as well as exposure to alternative green processes with recyclable reagents.
3:50 PM - 5:30 PM Sooner A

S11: Inorganic Chemistry
Chair and Presider: Doug Powell (Department of Chemistry & Biochemistry, University of Oklahoma)

3:50 T76 Synergism in the Flame Retardancy of Guanyl Urea Phosphate and Boric Acid Mixture on Polyurethane Foam.

4:10 T77 Synthetic and Mechanistic Studies of Migratory Insertion of CO into Cationic Methylpalladium Complexes Containing bis N-Heterocyclic Carbene (bis-NHC) Ligands

3:50 T76: Synergism in the Flame Retardancy of Guanyl Urea Phosphate and Boric Acid Mixture on Polyurethane Foam.

Presenter: Bhawani Regmi, Chemistry, Oklahoma State University

Authors and Affiliation: Bhawani Regmi and Dr. Allen Apblett, Oklahoma State University Chemistry Department Stillwater, OK 74078

There is a high demand for environmentally friendly, non-corrosive, and non-hygroscopic fire retardants to replace the commonly used compounds that have been found to have negative effects on human health and the environment. Previously, guanyl urea phosphate (GUP) was shown to work synergistically with boric acid to provide fire retardancy for wood. We have determined that GUP and boric acid interact with each other in aqueous solution, enhancing the solubility of boric acid, facilitating the use of an aqueous impregnation process. However, as the solution is dried the GUP and boric acid separate into the individual compounds so that their fire retardant properties come from the action of the individual components. The GUP/boric acid mixture was found to be an excellent non-hygroscopic flame retardant and smolder retardant when applied to carbon-loaded polyurethane foam. The thermal behaviors of samples were studied by thermogravimetric analysis (TGA) in air and found the synergistic behavior of GUP and boric acid mixture on flame and smolder retardancy.

T77: Synthetic and Mechanistic Studies of Migratory Insertion of CO into Cationic Methylpalladium Complexes Containing bis N-Heterocyclic Carbene (bis-NHC) Ligands

Presenter: Sri Subramanium, Chemistry, Oklahoma State University

Authors and Affiliation: Sri S. Subramanium and LeGrande M. Slaughter* Department of Chemistry Oklahoma State University Stillwater OK 74078

Methylpalladium complexes of bulky bis N-heterocyclic carbenes (bis-NHC), Pd(bis-NHC)(CH3)2 (1), have been synthesized from bisimidazolium salt, KOtBu and Pd(TMEDA)(CH3)2, where bis-NHC = 1,1′-dimesityl-3,3′-methylenebridimide-2,2′-diylidene (1a, DIMesMe), 1,1′-dimesityl-3,3′-ethylenedimide-2,2′-diylidene (1b, DIMesEt) and 1,1′-dimesityl-3,3′-propylenedimide-2,2′-diylidene (1c, DIMesPr).

Treatment of 1a-c with CH3I produced Pd(bis-NHC)(CH3)(I) (2a-c) and reaction of 2a-c with AgBF4 in CH3CN produced cationic [Pd(bis-NHC)(CH3)(NCCH3)][BF4] (3a-c). Molecular structure of the DIMesMe complex (3a) was determined, but the DIMesEt analogue (3b) was only stable at low temperature (< 0°C) and the DIMesPr complex (3c) was even unstable at -35°C. Reaction between 3a and CO produced [Pd(DIMesMe)(COCH3)(CO)][BF4] (4a) and its molecular structure was determined, providing the first such example of a methyl carbonyl Pd-NHC complexes. Treatment of 4a with excess CO produced [Pd(DIMesMe)(COCH3)(CO)][BF4] (5a), which was characterized using 1H NMR, 13C NMR and IR spectroscopy. The observed rate constant (kobs), at -50°C, for conversion of 4a to 5a was 1.18(2) x 10^-4 s^-1 at 1 atm of CO and 1.18(2) x 10^-4 s^-1 at 0.5 atm of CO. This carbonylation reaction was reversible and equilibrium data were determined from 4 to 25°C, giving thermodynamic parameters of ΔH° = -17(1) kcal mol^-1 and ΔS° = -42(4) cal mol^-1 K^-1 from the Vant’s Hoff plot. Kinetic and thermodynamic data for other complexes were also investigated.
T78: Crystallographic Analysis of Organometallic Structures with Extended Metallophilic and Pi-Pi Interactions

**Presenter:** LeGrande Slaughter, Chemistry, Oklahoma State University

**Authors and Affiliation:** LeGrande M. Slaughter (Corresponding, Presenting), Department of Chemistry, Oklahoma State University; Ilya M. Sluch, Department of Chemistry, Oklahoma State University; Anthea J. Miranda, Department of Chemistry, Oklahoma State University

Metallophilic interactions are weak bonds between d^8, d^10, and s^2 metal ions that can lead to extended chains of metal atoms in the crystalline state. In this study, a series of palladium and platinum isocyanide complexes of the type cis-M(CNAr)_2Cl_2 were structurally characterized by X-ray crystallography, revealing metallophilic interactions that ranged from dimer formation to infinite chain structures depending on the nature of the aryl substituents. These metallophilic interactions were in synergy with various aryl pi-pi interactions, with the dominant type of interaction apparently dependent on both electronic and steric properties of the isocyanides. Surprisingly, some of the compounds adopted structures with vacant or solvent-filled channels, apparently to maximize the synergy of metallophilic and pi-pi interactions. For the phenylisocyanide complexes, conditions were found by which different polymorphs of the same compounds containing either isolated dimers or extended metallic chains with attendant channels could be selectively obtained. For the platinum complexes, extended chain polymorphs were luminescent while the isolated dimer structures were not. The presence of extended metal-metal chains also appeared to correlate with the presence of twinning (pseudo- or non-merohedral) in the crystals.

T79: Light-Induced Transformation of Nanostructured V_2O_5·H_2O to V_2O_5

**Presenter:** C. Ozge Topal, Department Of Mechanical And Aerospace Engineering, Oklahoma State University

**Authors and Affiliation:** C. Ozge Topal and A. Kaan Kalkan, Functional Nanomaterials Laboratory, School of Mechanical and Aerospace Engineering, Oklahoma State University, Stillwater, OK 74078.

In the present work, light-induced phase transformation of a transition metal oxide has been observed and studied. This phase transformation occurs between two different oxides of vanadium, prepared by sol-gel chemistry, namely from V_2O_5·H_2O to V_2O_5 under laser irradiation (514 nm) as low as ~0.31 kW/cm^2. V_2O_5·H_2O to V_2O_5 transformation was studied by Raman spectroscopy in both air and Ar ambient. An interesting feature of this phase transformation is found to be its athermal origin. Raman spectroscopy was employed to rule out the heating effects and measure the temperature during the transformation which is as low as 25-29 °C (i.e., measurements performed at room temperature). In contrast, it was observed that the same transformation occurs at 350 °C when it is driven thermally by annealing samples for 10 minutes. Further, the present work explored kinetics of the light-induced V_2O_5·H_2O to V_2O_5 transformation by photoluminescence. The kinetics suggests either 1D nucleation and growth from predetermined nucleation sites or a photochemical reaction without nucleation.

T80: Silica Gel Supported Titanium Catalyzed Conversion of Benzyl Phenyl Ketone and Diphenylacetylene to Benzaldehyde.

**Presenter:** Robert Cannon, Chemistry, Oklahoma State University

**Authors and Affiliation:** Robert C. Cannon and Allen Apblett

Catalysts have a wide variety of application in chemistry and serve as the bases of many of the industrial synthesis of synthetic chemicals today. A catalyst was prepared using a titanyl sulfate and sulfuric acid solution and then coated on coarse silicon dioxide as a support. The titanium coated silica gel was used as a catalyst to convert both benzyl phenyl ketone and diphenylacetylene to benzaldehyde. In the process multiple intermediates are formed including benzil and benzyl phenyl ketone in the case of diphenylacetylene. This discussion will cover the kinetics, possible reaction pathways, and the reaction of other related compounds with this titanium catalyst.
3:50 PM - 5:30 PM Ballroom A
S4: Nanotechnology - Materials
Chair and Presider: Donna Nelson (Chemistry & Biochemistry, The University of Oklahoma)

3:50 T81 Strength Improvement via Coating of a Cylindrical Hole by Layer-by-Layer Assembled Polymer Particles
Presenter: Brian Grady, Chemical, Biological and Materials Engineering, University of Oklahoma
Authors and Affiliation: Nicholas Rupert, Brian Grady, University of Oklahoma
Gary Funkhouser, Halliburton Inc.

Negatively charged colloidal poly(methyl methacrylate-co-butyl acrylate) (P(MMA-BA)) particles, and positively charged dissolved poly(ethyleneimine) (PEI) were adsorbed onto a cement block using a layer-by-layer (LBL) assembly technique. The block was fashioned so as to have a cylindrical hole running from one face to another along the long axis of the rectangular block, and a fluid containing either of the two charged materials was pumped through the block. The result was a film tens of micrometers thick, and the pressure required to crack the cement block was measured after sealing one end of the hole. Latex particles with a Tg near the use temperature showed the maximum improvement in the cracking stress of the blocks. In a multilayer coating with identically sized particles, the cracking stress of the blocks increased to an improvement of 25% and then dropped off with increasing number of layers, even though the relationship between film thickness and the number of layers was linear. An improvement of about 30% in the cracking stress of the coated blocks was obtained when using multiple layers with different particle sizes. The effects of the number of layers and particle size on the cracking stress suggest that both the morphology and the thickness of the film play a role in performance. Tests done under confinement, e.g. with an external stress applied to the outside of the blocks, suggest that not only does a film-forming mechanism contribute to performance, but filling of microcracks in the rock may also play a role.

T82: Nanowire-Nanoparticle Conjugate Photolytic Fuel Generators
Presenter: Kaan Kalkan, Mechanical and Aerospace Engineering, Oklahoma State University
Authors and Affiliation: A. Kaan Kalkan, Sean MacLaskey, and Ryan Bogle, Functional Nanomaterials Laboratory, Department of Mechanical and Aerospace Engineering, Oklahoma State University, Stillwater, OK 74078

Conversion of sunlight to chemical fuels by artificial photosynthesis has been a long-sought goal. The present work demonstrates a hydrogen generating photolytic device, which consists of a low band gap oxide semiconductor nanowire decorated with metal nanoparticles. The nanostructures are synthesized via sol-gel and reduction chemistries, respectively, allowing a low-cost technology. The technology also aims at high photolytic conversion energy and stability by making use of multifunctional nanostructures with unique electronic, photonic, and plasmonic attributes at the nanoscale. Our preliminary work has proven a reproducible quantum efficiency of 79% under 425 nm excitation. Extinction spectrum of Au nanoparticle-decorated nanowires show multiple resonances (i.e., 420, 475 nm) with no coincidence with the localized surface plasmon resonance for nanoparticles (i.e. 530 nm). We attribute these new resonances to coupling of light to nanowire waveguide modes in the direction of nanowire axis, enhancing the optical absorption. Under investigation is possible ballistic (i.e., “collisionless”) transport in the semiconductor nanowires whose impact is expected to be efficient channelling of photogenerated electrons and holes to their respective redox reactions.

T83: Silica Incorporated Titania Semicoducting Nanoparticles: Transmission IR Studies towards Photocatalysis
Presenter: Dilip Paul, Chemistry, Pittsburg State University
Authors and Affiliation: Dilip K. Paul Chemistry Department, Pittsburg State University, Pittsburg, KS 66762

Silica Incorporated Titania metal oxide nanoparticles were synthesized by the sol-gel process. These TiO2-SiO2 nanoparticles exhibit different photochemical properties from TiO2 itself. The adsorption of 2-CEES, acetaldehyde and 2-butenal have been studied by molecularly sensitive FT-IR. The oxidation reaction of the above molecules carried out under both dark and UV light conditions. The oxidation product of aldehyde may result in the formation of corresponding acid and carboxylate species. Detailed analysis of infrared data has been used to investigate the products and the kinetics of photochemical oxidation reactions for both thiol and aldehydes.

[ ABSTRACTS ]

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T84: Electrochemical Characterization of SnO2 Nanobasket Electrodes with Capacities Exceeding Theoretical Values

**Presenter:** Matthew Smith, Department of Chemistry and Biochemistry, University of Tulsa

**Authors and Affiliation:** Matthew Smith, Paige Johnson, Dale Teeters

Our lab has shown that nanoporous membranes can serve as templates for RF magnetron sputtering, which results in novel self-assembled structures termed “nanobaskets.” These capped cylindrical structures show a drastically increased surface area and, subsequently, would lead to enhanced electrode performance; specifically: higher capacities and better cyclability. Furthermore, these nanobaskets have been shown to be constructed of an even smaller nanoparticle substructure that further increases the surface area and performance of the electrode. The purpose of this work was to characterize and gain a better understanding of the structure, mechanisms and electrochemical properties of SnO2 nanostructures as applied to nanoscale battery technology.

Samples were analysed via cyclic voltammetry, galvanostatic charge-discharge experiments, and scanning electron and atomic force microscopy. Cross-sectional analysis performed via SEM-FIB.

Our data shows that the fully nanostructured SnO2 possesses discharge capacities as high as 1730 mAh/g and maintaining over 72% initial discharge capacity after 9 cycles. This is more than twice the theoretical capacity of 781 mAh/g for bulk SnO2. We attribute this drastic increase above the theoretical value to interfacial storage of lithium between the nanoparticle substructure in the nanobaskets. This phenomenon has the potential to greatly increase the performance of SnO2 electrode material.

T85: Nanotechnology for Neutralization of Explosives in the Field and the Laboratory

**Presenter:** Allen Apblett, Chemistry, Oklahoma State University

**Authors and Affiliation:** Allen Apblett, Nicholas Materer, Kevin Barber, and Derek Bussan. Department of Chemistry, Oklahoma State University, Stillwater, OK

Both improvised explosives and conventional explosives pose an increasing threat world-wide due to military and terrorist activities. We have developed solutions based on nanotechnology that can be used to neutralize unexploded ordnance in situ or to destroy outdated munitions. These reagents can also be used to neutralize the peroxide-based explosives such as hexamethylenetriperoxidediamine (HMTD) and triacetone triperoxide (TATP) that are favored by terrorists. Chemists often face risks daily from similar explosives that form spontaneously in organic solvents. Our technology can also be used to prevent build-up of peroxides in laboratory solvents. For this application, the reagent does not contaminate the solvent and provides a simple colorimetric indication that the solvent is still safe to use.
ABSTRACTS

3:50 PM - 6:00 PM Ballroom C
S12: Pharmacology/Natural Products
Chair and Presider: Robert Cichewicz
(Chemistry & Biochemistry, The University of Oklahoma)

3:50  T86  Biosynthesis of Glycosides - Glycosyltransferase Structures and Engineering

4:10  T87  Metabolomics and Integrated Functional Genomics Reveal Novel Information Related to Medicago Secondary Metabolism

4:30  T88  Chemical Epigenetic Manipulation of Secondary Metabolite Production by a Penicillium citreonigrum Isolate Obtained from the Atlantic Forest

4:50  T89  Naturally-Occurring Triterpenoids as Potential Anticancer Agents: Prevention and Treatment of Colorectal Cancer

5:10  T90  Anti-Cancer Action of Frankincense Oil from Boswellia species

5:30  T91  Dried Plum Extract Reverses Osteopenia by Altering Osteoblast and Osteoclast Differentiation and Activity

T86: Biosynthesis of Glycosides - Glycosyltransferase Structures and Engineering
Presenter: Xiaoqiang Wang, Plant Biology Division, Noble Foundation
Authors and Affiliation: Xiaoqiang Wang, Hui Shao, Lenong Li, Luis L. Escamilla-Trevino, Luzia Modolo, Xianzhi He, Jack W. Blount, Lahoucine Achnine, Richard A. Dixon; Plant Biology Division, Samuel Roberts Noble Foundation, 2510 Sam Noble Parkway, Ardmore, OK 73401, USA

A large portion of bioactive natural products are glycosides attached with sugars. Various glycosides are synthesized in plants and microorganisms, and uridine diphosphate glycosyltransferases (UGTs) are key players in the biosynthesis of glycosides. UGTs specifically utilize UDP-sugars as donors and transfer various sugars to plant natural products. We determined structures of three UGTs from Medicago truncatula. These structures revealed the detailed structural features of plant UGTs and interactions between enzymes and substrates, which define the substrate specificity of individual enzymes and provide structural bases for understanding the catalytic mechanism of glycoside biosynthesis. Structure-based UGT enzyme engineering was carried out to explore the roles of key residues involved in substrate binding and enzyme activity. Substitutions in the substrate binding pocket can alter substrate specificity and product regioselectivity; compromise or enhance catalytic efficiency; and confer reversibility to the glycosylation reaction. UGTs are very promising tools for manipulating glycosylation patterns to generate novel bioactive glycosides or for designing effective mutants with reversibility to synthesize activated sugars.

T87: Metabolomics and Integrated Functional Genomics Reveal Novel Information Related to Medicago Secondary Metabolism
Presenter: Zhentian Lei, Plant Biology Division, The Noble Foundation
Authors and Affiliation: Zhentian Lei, Mohamed A. Farag, Corey D. Broeckling, David V. Huhman, Ewa Ubanczyk-Wochniak, Wensheng Li, Mohamed Bedair, Bonnie S. Watson, Marina Naoumkina, Bettina Deavours, Richard A. Dixon, Lloyd W. Sumner; The Samuel Roberts Noble Foundation

Legumes are a fundamental food source for most global cultures due to their high protein contents achieved through symbiosis with nitrogen-fixing rhizobia. They also produce a wide array of natural products that play critical roles in plant disease/defense responses and are important to human and animal health. These include the flavonoids, isoflavonoids, and saponins which serve as key signaling molecules in plant-microbe interactions, as primary defense compounds, and increasingly as important nutraceuticals and pharmaceuticals. Medicago truncatula, a close relative of the premium and global forage legume alfalfa (Medicago sativa), is an ideal model legume for the study of legume biology due to the availability of a near complete genome sequence and a 61,200 probe set Affymetrix GeneChip for DNA microarray analyses. Unfortunately, the application of such molecular tools to the study of plant secondary metabolism is currently limited by deficient and/or inaccurate annotation of secondary metabolic genes and enzymes. Metabolomics is an important part of systems biology approach which provides a powerful platform for the discovery and hypothesis driven assessment of metabolic networks. This presentation will provide specific examples of how Medicago truncatula metabolomics is yielding novel discoveries and mechanistic insights related to Medicago secondary metabolism.
T88: Chemical Epigenetic Manipulation of Secondary Metabolite Production by a *Penicillium citreonigrum* Isolate Obtained from the Atlantic Forest

**Presenter:** Xiaoru Wang, Chemistry and Biochemistry, University Of Oklahoma

**Authors and Affiliation:** Xiaoru Wang, José G. Sena Filho, Ashley R. Hoover, Jarrod B. King, Trevor K. Ellis, Douglas R. Powell, Robert H. Cichewicz; Natural Products Discovery Group, Department of Chemistry and Biochemistry, 620 Parrington Oval, Room 208, University of Oklahoma, Norman, Oklahoma, 73019-3032, USA.

Chemical epigenetics is proving to be a very powerful tool for inducing the production of structurally unique secondary metabolites from fungi. In this study, we have applied this methodological approach to the screening of a *Penicillium citreonigrum* isolate obtained from the Atlantic Forest. This region is regarded as one of the most species-rich, but highly endangered habitats in the world today. Application of the DNA methyltransferase inhibitory agent 5-azacytidine to the fungus resulted in the significant diversification of the organism’s secondary metabolite profile. The effects of the chemical epigenetic modifier were readily apparent in the substantial change that occurred in the fungal guttate, which changed from its normal clear to dark red. An investigation of the newly excreted compounds resulted in the identification of six azaphilones, pencolide, and two new meroterpenes that we have named atlantinones A and B. The structures of the new metabolites along with their antimicrobial activities will be discussed.

T89: Naturally-Occurring Triterpenoids as Potential Anticancer Agents: Prevention and Treatment of Colorectal Cancer

**Presenter:** Chinthalapally Rao, Medicine, Oklahoma University Health Sciences Center, Oklahoma City, OK

**Authors and Affiliation:** Rao, C.V., Jagan Patlolla, Naveena, B. Janakiram. Authors Affiliated to: Department of Medicine, Hem-Onc Section, University of Oklahoma Health Sciences Center, Oklahoma City, OK-73104

Epidemiologic and laboratory studies have shown that chronic disease preventing properties are widely distributed in number of naturally-occurring products such as fruits, vegetables and sea foods. In the past and recent years, number of chemical molecules derived from natural sources are established as potential anticancer agents. Most of these anticancer agents are chemically diverse and belong to different classes of chemical structures. Triterpenoids are one such group of natural agents, which have potential applications for the prevention and treatment of not only cancer, but also of many other diseases associated with inflammation.

Recently, a renewed interest has increased in identifying potential triterpenoids for cancer prevention and treatment. We have identified and tested several triterpenoids from different natural sources as effective colon cancer inhibiting agents using preclinical animal studies. Triterpenoid agents like β-escin (derived from Horse Chest nut), oleanolic acid (ONA) (leaf of *Olea europaea* L.) and its analog 18α-olean-12-ene-3β-23,28-triol (OT), a mixture of ursoic acid, betulinic acid, oleanolic acid (isolated from almond husk) and frondosides (isolated from a sea cucumber) are tested in well established models of colon cancer. In chemically-induced rat colon carcinogenesis model, 250 ppm and 500 ppm β-escin in diet, significantly suppressed occurrence of preneoplastic lesions by 50% (p < 0.0001); and multicrypt lesions by 65% (p< 0.0001). Similarly, 750 ppm and 1,500 ppm ONA and 250 and 500 ppm OT suppressed occurrence of carcinogen-induced rat colonic preneoplastic lesions (36–52% p<0.01 to p<0.001), and multicrypt aberrant crypt foci’s (47–67%, p<0.001- p<0.0001). Importantly, sea cucumber extract (150 ppm and 450 ppm in diet) containing frondosides suppressed colonic lesion occurrence by 34% to 55% (p< 0.01 to p< 0.0001) and multicrypt lesion formation by 48-70%, (p< 0.0001). It is note worthy that mixture of ursoic acid, betulinic acid, oleanolic acid, fed in diet (200 mg/Kg) significantly inhibited development of colon adenocarcinomas in rat. In this bioassay, rats fed triterpenoids extracted from almond husk were found to significantly reduce colon adenocarcinoma incidence (43%, p<0.001) and multiplicities (~64%, p < 0.0001). Furthermore, triterpenoids possess significant ability to suppress proliferation (decrease in PCNA), and induction of apoptosis in human colon cancer cells. Molecular targets of triterpenoids include COX-2, iNOS, p21^WAF1/CIP1 and cyclin B1. Taken together, both preclinical cancer bioassays and mechanistic data clearly suggest potential usefulness of naturally occurring triterpenoids for colorectal cancer prevention and treatment.
T90: Anti-Cancer Action of Frankincense Oil from *Boswellia* species  
**Presenter:** Hsueh-Kung Lin, Urology, University of Oklahoma Health Sciences Center  
**Authors and Affiliation:** Departments of Urology and Physiology University of Oklahoma Health Sciences Center  

Originating from Africa, India, and the Middle East, frankincense has been important both socially and economically as an ingredient in incense and perfumes for thousands of years. Frankincense resin is obtained by tapping *Boswellia* trees, and has been considered throughout the ages to have a wealth of health supporting properties. The resins of *Boswellia* species have been used for the treatment of rheumatoid arthritis and other inflammatory diseases through their proposed anti-inflammatory activity. Chemical extracts of frankincense resins have also been shown to possess anti-cancer activities in many types of cancer cells. Frankincense oil prepared from steam distillation of frankincense resin for aromatherapy was examined for its anti-cancer activity against human bladder cancer cells. Within a range of concentrations, frankincense oil specifically suppressed cell viability in bladder transitional carcinoma J82 cells but not in immortalized normal human UROtsa cells. Comprehensive gene expression analysis confirmed that frankincense oil activates genes that are responsible for cell cycle arrest, cell growth suppression, and apoptosis in J82 cells. In an orthotopic mouse bladder cancer model, frankincense oil suppressed bladder cancer progression through a combination of suppressed tumor cell growth and elevated tumor cell death. Although boswellic acids have been shown as the major component in chemical extracts of frankincense resins for anti-cancer activity, frankincense oil does not contain detectable boswellic acids. The active component that is responsible for anti-cancer activity of frankincense oil remained unidentified. However, frankincense oil might represent an alternative intravesical agent for bladder cancer treatment.

T91: Dried Plum Extract Reverses Osteopenia by Altering Osteoblast and Osteoclast Differentiation and Activity  
**Presenter:** Brenda Smith, Department of Nutritional Sciences, Oklahoma State University  
**Authors and Affiliation:** Brenda J. Smith, Yan Wang, Elizabeth Rendina, Edralin A. Lucas; Department of Nutritional Sciences, Oklahoma State University, Stillwater OK  

Previously, we have reported that dietary supplementation with dried plums (*Prunus domestica* L.) reverses bone loss in animal models of osteoporosis. These improvements in skeletal health are characterized by increased bone density and the restoration of trabecular bone microarchitecture and biomechanical properties. The capacity of dried plum to reverse bone loss is unique among the currently available treatment options and has been attributed in part to its polyphenolic components. Initial studies in animal models demonstrated that a crude extract of dried plum’s polyphenols accounted for approximately 75% of the effect of the dried plum on bone. Subsequent *in vitro* studies have shown that the dried plum extract increases osteoblast activity and calcified nodule formation. This improved osteoblast function was associated with the up-regulation of key transcription factors involved in osteoblast differentiation, growth factors, and enzymes involved in collagen crosslinking in bone. Additionally, the dried plum extract down-regulated the catabolic activity of osteoclasts by inhibiting their differentiation. The results of these *in vitro* studies suggest that the dried plum extract favorably affects the cells that regulate the catabolic and anabolic activity in bone. More recently, *in vivo* studies have demonstrated that when the extract was combined with two other nutrients found in dried plum, the effects on bone mass and microarchitecture were comparable to that of the whole dried fruit. Ongoing studies designed to identify the bioactive component(s) in the extract are underway in our laboratory.
**POSTER ABSTRACTS**

8:30 AM - 5:00 PM Ballrooms H and I
Analytical/Physical Chemistry – Poster

**P1: Adsorption and Reaction of Propene on Different Cationic Forms of Y Zeolite: Prediction of Polymerization Activity from IR Molar Absorption Coefficients.**

*Presenter: Kassie (ThuHuong) Ngo, Chemical, Biology and Materials Engineering, The University of Oklahoma*

*Authors and Affiliation: ThuHuong Ngo(a), Jutta Kröhnert(b), and Friederike C. Jentoft(a) (a)Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK 73019, USA. (b)Department of Inorganic Chemistry, Fritz Haber Institute, Max Planck Society, 14195 Berlin, Germany.*

Absorption bands of molecular vibrations in infrared spectra are characterized by their position, shape, and intensity. The frequency shift of vibrations that results from adsorption on a catalyst surface has been widely used to interpret bond strength variations; however, the intensity of absorption bands has not been extensively analyzed. The intensity of IR stretching bands depends on the change in dipole moment during vibration. If a bond is polarized (and thus activated for a heterolytic bond cleavage) through adsorption on a catalyst, the molar absorption coefficient of the corresponding band should increase. In this work, we seek to establish a correlation between the reactivity of the C=C bond of propene and the molar absorption coefficient of the C=C vibration. The interaction of propene with a series of cation-exchanged faujasites (zeolite Y) was investigated. The C=C bond absorption coefficients increase in the order NaY < CaY < MgY. Our results show that higher molar absorption coefficients for the C=C vibration of adsorbed propene correlate to polymerization activity at lower temperature. These findings demonstrate the potential of the IR band intensity to predict catalytic activity.

**P2: Analysis and Quantitation of Phthalate Plasticizers in Surface Waters Using SPME/GC-MS**

*Presenter: Basil Mathews, Chemistry, University of Central Oklahoma*

*Authors and Affiliation: Goode, Sharome; Mathews, Basil; Thomas, Wesley. John Bowen, University of Central Oklahoma, Department of Chemistry, Edmond, OK 73034*

Water from treatment plants is treated to eliminate pathogens but not harmful chemicals. The water from these treatment plants is discharged into surface waters after treatment. It is known that harmful chemicals are released, but these have not been quantitated to reveal the impact it causes on the environment. Plasticizers, a known endocrine disrupter, are believed to be one of the chemicals released by these treatment plants. This study is used to measure the occurrence of phthalate plasticizers in surface waters using a SPME fiber. The SPME fiber is used to adsorb these dilute compounds in order to be identified. Water samples were taken from the Veonalia Treatment Center to analyze the distribution of phthalate plasticizers in source waters. Analytes were adsorbed onto the SPME fiber and then desorbed by the injection port of the GCMS. The GCMS allowed the separation of the analytes in order for proper identification and quantitation. Dimethyl phthalate was used as an internal standard. Our data showed that detectable concentrations of phthalates like dimethyl phthalate and dibutyl phthalate did exist at surface water locations. We deem that some sort of regulations need to be placed on treatment plants in order to prevent such adverse affects.

**P3: Catalytic Isomerization of n-Butane on H-Mordenite: Influence of Hydrogen Partial Pressure**

*Presenter: Matthew Wulfers, Chemical, Biological, & Materials Engineering, University of Oklahoma*

*Authors and Affiliation: Matthew J. Wulfers, Friederike C. Jentoft Chemical, Biological, and Materials Engineering, University of Oklahoma, Norman, OK 73019, USA*

Catalytic skeletal isomerization of n-butane is valuable for production of isobutane and isobutene, used in alkylation and methyl tert.-butyl ether production, respectively. Currently used platinum-doped chlorided alumina catalysts are candidates for replacement because of their corrosive nature and potential process hazards. Zeolites such as H-Mordenite and solid oxides such as sulfated zirconia are highly acidic and thus capable of performing this difficult reaction. These catalysts have the advantage that they are tolerant to contaminants, regenerable, and perform at low temperatures which thermodynamically favor isobutane at equilibrium. However, both catalysts suffer from deactivation and require platinum doping and hydrogen addition to the feed to stabilize performance.

In this study we have varied the hydrogen partial pressure during n-butane isomerization on both parent and platinum-doped H-Mordenite. Multiple temperatures and hydrogen partial pressures were investigated, allowing for calculation of activation energies of isobutane and unwanted side products such as propane and isopentane. The catalytic performance is stable above a critical H2 pressure; however, the activity decreases with increasing H2 partial pressure. In situ ultraviolet-visible spectroscopy allows for monitoring of the accumulation of unsaturated allylic species on the catalyst surface. The formation of unsaturated species coincides with deactivation, indicating poisoning of active sites.
P4: Charge-Transfer Mediated Photocemistry of Small-Ring Systems.
**Presenter:** Paritosh Das, Physical Sciences, Cameron University
**Authors and Affiliation:** Sweta Shrestha and P. K. Das, Physical Sciences Department, Cameron University, Lawton, OK 73505.

We are interested in mechanisms of chemistry, particularly, ring-opening, of small-ring systems through photo-induced charge transfer interactions. In this poster, we will present results from our studies of the quenching of steady-state fluorescence of two cyanoaromatics, namely, 1,4-dicyanonaphthalene (DCN) and 9,10-dicyanoanthracene (DCN) by cis- and trans-stilbene oxides, cis-triphenyl aziridine, and several aromatic amines and phenols. In particular, in acetonitrile, cis-triphenylaziridine has been found to quench both DCN and DCA fluorescence efficiently with diffusion-controlled rates comparable to those for quenching by amines and phenols. In contrast, as fluorescence quenchers, cis and trans-stilbene oxides are poor for DCA and modest for DCN.

P5: Correlation of Hydrogen Bonding Species in N,N'-DMEDA and N,N'-DMPDA and Their Complexes with Lithium Trifluoromethanesulfonate with Infrared and Raman Vibrational Band
**Presenter:** Rachel Mason, Chemistry & Biochemistry, University of Oklahoma
**Authors and Affiliation:** Rachel N. Mason and Roger E. Frech; Department of Chemistry and Biochemistry, The University of Oklahoma, Norman, Ok, 73019

Vibrational signatures of polymeric systems can be complex and difficult to interpret confidently without significant prior knowledge of the structure and/or interactions occurring in the system. By employing small organic molecules that mimic the structure and behavior of given aspects of the polymeric system, insight into the complex nature of the system can be acquired. In the present work, N,N′-dimethylethylendiamine (N,N'-DMEDA) and N,N′-dimethylpropylenediamine (N,N'-DMPDA) were utilized to model poly(ethylenimine), PEI, and poly(propyleneimine), PPI, in an effort to understand the hydrogen bonding interactions occurring in the polymers.

Both N,N'-DMEDA and N,N'-DMPDA are known to experience hydrogen bonding at the amino nitrogens. Hydrogen bonding results in a change in the strength of the N-H bond, which is reflected in a shifted frequency of the NH stretching band (νNH) in both infrared (IR) and Raman spectra. To correlate the band frequency with the hydrogen bonding species IR and Raman spectra, were collected for the neat model compounds and model compounds diluted in carbon tetrachloride (CCl4) over the range of 1:2 to 30:1 mole ratio of CCl4 carbon to model compound nitrogen (C:N). Further, spectra from complexes of the model compounds and lithium trifluoromethanesulfonate (LiTf) were also obtained for the neat complexes and the complexes diluted in CCl4.

Examination of the nNH mode resulted in the identification of six different NH species: non-hydrogen bonded NH, intermolecularly hydrogen bonded NH, singly intramolecularly hydrogen bonded NH, n-mer type hydrogen bonded NH, dually intramolecularly hydrogen bonded NH, and Li+ associated NH.

P6: Developing Surfactant Formulation for Oil-Wet Carbonate Formations
**Presenter:** Oluwafemi Afelumo, Petroleum Engineering, University of Oklahoma
**Authors and Affiliation:** Oluwafemi Afelumo, Bor-jier Shiau, Jeffrey H. Harwell Applied Surfactant Laboratory (ASL), University of Oklahoma 100 East Boyd Street, Sarkey’s Energy Center, Norman, Ok 73019

There is growing need for developing efficient means of enhancing oil recovery from mature fields already produced through primary especially because very few new fields are being discovered. Surfactant flooding is one of such means of enhancing oil recovery. This technology is useful in oil-wet formations. The target characteristics for a good surfactant formulation are; ability to form winors type III microemulsion, low interfacial tension between oil and water, no precipitation, and reasonable low adsorption. However, most of the surfactants used for this process are anionic surfactants. These present a problem when applying them to carbonate formations because the positively charged formations cause heavy adsorption of the anionic surfactants which are negatively charged. Cationic surfactants present a solution to this problem because they are positively charged and therefore would not adsorb readily on positively charged surfaces. A formulation that is a mix of cationic (predominantly) and anionic surfactants is developed in order to satisfy the characteristics for a formulation that can be used in carbonate formations. The formulation developed shows results that are favorable for use in enhancing oil recovery.

P7: Differential Pulse Anodic Stripping Voltammetry (DPASV) for the Detection of Barium from Oil Well Water
**Presenter:** Crystal Mars, Chemistry and Physics, Southwestern Oklahoma State University
**Authors and Affiliation:** Crystal Mars and Dr. Curt Woolever, Department of Chemistry and Physics, Southwestern Oklahoma State University, Weatherford, OK 73096

Differential Pulse Anodic Stripping Voltammetry (DPASV) has been applied for quantitative determination of Barium (Ba) from oil well water samples. These oil well water samples are from Oklahoma wells that have been under waterflood. The use of different concentrations of lithium perchlorate (LiClO4) and different DPASV parameters, such as pulse amplitude and scan rate, are being investigated for qualification and quantitation of Ba from these samples.
P8: Environmental and Galvanic Corrosion Rates for Iron and Zinc Wires  
**Presenter**: Ahmad Razzaghi, Chemistry, Oklahoma State University  
**Authors and Affiliation**: Ahmad Razzaghi, Dane Scott, Kevin Barber, Allen Apblett and Nicholas Materer, Department of Chemistry, Oklahoma State University

Millions of dollars are lost each year because of corrosion induced damage, a large percentage from the corrosion of iron and steel. Corrosion is the electrochemical oxidation of metals with an oxidant such as oxygen. The rate of corrosion can be enhanced in a salt solution. Using wires as a model, the corrosion of iron and zinc wires was studied in 5% NaCl solutions. When two types of metals are in electrical contact via an electrolyte, one of them will corrode preferentially due to difference in electrode potential of these metals. his type of corrosion is called galvanic corrosion. The galvanic corrosion rate for zinc wires attached to iron coupons in NaCl solution was also measured and compared to rate of zinc corrosion found for the NaCl solution. These corrosion rates can be used make a corrosion sensor.

P9: Evaluation of Water Repellency on Cotton Fabric Using Contact Angle Measurements  
**Presenter**: Srinivas Hanumansetty, Chemical Bio And Materials Engineering Department, University Of Oklahoma  
**Authors and Affiliation**: Rachel Weber, Department of Chemical Engineering, University of Oklahoma, Norman, Oklahoma 73019 Srinivas Hanumansetty, Department of Chemical Engineering, University of Oklahoma, Norman, Oklahoma 73019 Edgar A. O ‘Rear, Department of Chemical Engineering, University of Oklahoma, Norman, Oklahoma 73019

Common cotton textiles are hydrophilic in nature. Thin film fluoropolymer coating on cotton fibers of tens of nanometers thick gives the property of being water repellent. Here we report evaluation of water repellency of cotton fabric modified by admicellar polymerization using contact angle measurements. The water repellency evaluated by contact angle determination shows static contact angles as high as 140 or above. Various formulations have been tried and contact angles are measured with comparison to wetting times. Contact angles measurements allow assessment of durability of fabric with washing.

P10: H2O Proton Dissociation Energies of Zn(II) Complexes  
**Presenter**: douglas Linder, Chemistry and Physics, Southwestern Oklahoma State University  
**Authors and Affiliation**: Brett Baker and Douglas Linder, Department of Chemistry and Physics, Southwestern Oklahoma State University Weatherford, Oklahoma

H2O proton dissociation energies of several Zn(II) complexes have been calculated using density functional theory methods. Results will be discussed and relevance to biological proton transfer reactions will be set forth.

P11: Low Interfacial Tension (IFT) Surfactants Systems In High Salinity Conditions  
**Presenter**: Ovinuchi Anwuri, Petroleum Engineering, University of Oklahoma  
**Authors and Affiliation**: Ovinuchi Anwuri, David Paya, Bor-jier Shiau, Jeffrey H. Harwell, Applied Surfactant Laboratory (ASL), University of Oklahoma 100 East Boyd Street, Sarkey’s Energy Center, Norman, Ok 73019

There are growing interests in Enhanced Oil Recovery (EOR) technologies with the recent stability of oil prices and continual depletion of reserves. In this study, we are able to develop the surfactant candidates with characteristic of ultra-low Interfacial tensions (IFTs) and consequently good oil recovery without relying on formation of type III microemulsion. Previous studies showed that at higher surfactant concentrations we have a three-phase system and in lower surfactant concentrations (≤ 0.2%) we can have a two-phase system (Miller et al 1991). One-dimensional Sand Pack Column Studies using decane and crude oil samples retrieved from a local sandstone formation in Norman, Oklahoma, were then carried out using crushed Berea sandstone at reservoir temperature. The results were encouraging as about 40% of the remaining crude was recovered both by visual observation and final soil extraction. With the surfactant blend developed, with the aid of a co-solvent (IPA), we were able to show that we can achieve ultra-low interfacial tension in high salinity reservoirs at low surfactant concentrations, demonstrating a new approach to select the optimal surfactant for chemical flooding suitable for oil recovery.

P12: Quick decision Making for the Application of Surfactant Flooding in Oil Field  
**Presenter**: Piljin Moon, Petroleum Engineering, The University of Oklahoma  
**Authors and Affiliation**: Author: P.J. Moon, Univ. of Oklahoma Affiliation: Ben Shiau, Univ. of Oklahoma, Jeffrey Harwell, Univ of Oklahoma

Surfactant flood is one of the most effective methods to improve oil recovery. However, performance results of surfactant flooding in the laboratory can be different from results of field application because reservoir data are always limited in the reason of testing cost and stopping oil production. Therefore, it is required to express economic benefit with probability in order to make a decision for huge investment of surfactant process. Reservoir simulation can show one results under one condition. It is good to run reservoir simulation as many as possible to quantify uncertainties. However, it is not simple to say running simulation about 1000 cases because computing time and cost will be high. This difficulty will be overcome when Monte Carlo
simulation is applied in proxy equation. Proxy equation can be made with simulated results of experimental design by use of regression method. After proxy equation is proved to work properly instead of reservoir simulation, 1000 times of simulation can be run easily by commercial software, Crystal Ball. Based on those results, economic benefits are estimated quickly. In addition, sensitivity analysis from 1000 simulated results can contribute to find key factors that engineering should control to maximize the profit and minimize the risk.

P13: The Toxicology of Malathion in Select Blow Flies

Presenter: Mohammed Sheikh, Chemistry and Biochemistry, University of Oklahoma

Authors and Affiliation: Mohammed Osman Sheikh, University of Oklahoma, Department of Chemistry and Biochemistry

Our current research project will study the effects of common insecticides on blow flies (Diptera: Calliphoridae) based on previous research. Blow flies are important in the field of forensics for the determination of the postmortem interval (PMI) of a human or animal. The postmortem interval is the time between the death and discovery of a human or animal by an investigator (Buley 2008). Analyzing the life cycle of the flies can help determine the PMI, as they are among the first insects to arrive to and colonize a decomposing body. However, there is evidence that insecticides may have an impact on the life cycle of the Calliphoridae, thus potentially skewing PMI calculations and estimates. The insects could be exposed to the insecticides by either consuming the flesh of an individual that has committed suicide by means of ingesting the insecticide, or by contact exposure from a crime scene that insecticide has been applied to by a criminal in order to decrease the amount of insects present, therefore willfully intending to alter the PMI.

One common commercially available insecticide that has been noted to be used by suicide victims is malathion. Our research will focus on looking at the effects of malathion on the growth and development of the different species. If there is any evidence of malathion influencing the development of the Calliphoridae, then there would also be a correlation between the presence of malathion and its impact on PMI calculations, thus impacting forensic analysis. We will be using 0.01% malathion, administering the pesticide by absorbance into the food source. Bioaccumulation of malathion in the larvae will be determined by monitoring its concentration in the larvae at three different ages of the maggots. Gas chromatography with mass spectrometry will be used in the detection of malathion in respective samples of larvae.

P14: Altered Sensitivity to MDMA in Mice Made Tolerant to the Hallucinogen DOI

Presenter: Jacob Hostetler, Oral Roberts University

Authors and Affiliation: Jacob Hostetler, Oral Roberts University, Tulsa, OK; Dr. William Fantegrossi, University of Arkansas for Medical Sciences

Rationale: Dissimilarities have been reported in the limited number of studies that have directly compared the behavioral and pharmacological effects of the hallucinogen 3,4-methylenedioxyamphetamine (MDMA or “ecstasy”) and its enantiomers. While human drug abusers consume MDMA in its racemic form, the two distinct enantiomers of MDMA are each biologically active and may possess different behavioral and physiological actions. Behavioral tolerance is a phenomenon reasonably common among drugs of abuse. Hallucinogenic drugs, such as 2,5-dimethoxy-4-iodoamphetamine (DOI), seem to be particularly susceptible to the phenomenon. MDMA and its isomers are similar to DOI, both in terms of chemical structure and in pharmacological affinity for the serotonin 5HT2A receptor in the brain. The influences of prior hallucinogen exposure on MDMA effects are not known.

Objectives: The objective of this study was to assess the novel effects of S(+)-MDMA and R(-)-MDMA, and their combination as racemic MDMA, on sensitivity to thermoregulation and locomotor stimulation in mice made previously tolerant to DOI. Methods: Biotelemetry probes were surgically implanted into the gut of the test subjects and transmitted core temperature and locomotor activity data. A pretreatment of 10.0 mg/kg DOI was injected intraperitoneally once daily into each animal for three consecutive days. A challenge dose of either 10.0 mg/kg or 30.0 mg/kg MDMA was given on the fourth day. Test data collection commenced immediately after the MDMA dose was administered and continued for 24 hours. Results: DOI untreated mice challenged with a 10 mg/kg dose of MDMA exhibited hypothermic effects and recovered to baseline temperature within 60 minutes. Untreated mice that received a 30 mg/kg dose of racemic MDMA or S(+)-MDMA showed acute hyperthermia.

DOI pretreatment renders mice less sensitive to the effects of racemic MDMA on core temperature. DOI pretreatment contributes to more sensitivity to the effects of racemic MDMA on locomotor activity counts in mice. The S(+)-MDMA enantiomer yielded a definite effect on hyperthermia recovery. S(+)-MDMA presented a possible increase in sensitivity to locomotor stimulative effects. Conclusions: Results of this experiment suggest that behavioral tolerance to DOI alters sensitivity to the effects of racemic MDMA and its S(+) isomer. As a 5-HT2A agonist, DOI down-regulates the expression of this receptor. It also enhances locomotor activity induced by S(+)MDMA much like psychostimulant sensitization phenomena.
L-Lysine is an essential amino acid for humans and animals and can only be obtained through the diet. In bacteria, lower eukaryotes, and plants, lysine is synthesized via the diaminopimelate pathway (DAP). Fungi and euglenoids use the α-aminoadipate (AAA) pathway. An α-aminoadipate aminotransferase (AAAT) is thought to catalyze the fourth step in the α-aminoadipate pathway in yeast. The AAAT is pyridoxal 5'-phosphate (PLP)-dependent aminotransferase that catalyzes the interconversion of α-ketoacid and α-aminoacid, using glutamate as the amino donor. The S. cerevisiae genome has been completely sequenced. Extensive genetic, enzymatic, and regulatory studies of the lysine biosynthetic pathway are being carried out in S. cerevisiae. Seven genes, eight steps and more than 12 non-linked genes are responsible for the biosynthesis of lysine in yeast. The gene for AAAT in yeast has not yet been identified or cloned, thus nothing is known of the specific gene catalyzing the reaction, its substrate specificity or the details of its chemical mechanism with α-ketoacid and α-aminoacid as substrates. We have used sequence alignments and a homology search for conserved amino acid residues to identify six genes, which likely code for aminotransferases in Saccharomyces cerevisiae. Of these aminotransferases, the specific one which is involved in the lysine biosynthetic pathway has not been identified or characterized. The purpose of this project is to identify the enzyme α-aminoadipate aminotransferase involved in the lysine biosynthetic pathway in yeast and to characterize the enzyme using initial velocity, inhibition studies and pH rate studies.

P16: Cloning of CaSSK1, a Gene that Expresses an Oxidative Stress Protein from Candida albicans

**Presenter:** Hui Tan, Physical Sciences Dept., Cameron University

**Authors and Affiliation:** Steffan D. Sigler and Hui Tan, Department of Physical Sciences, Cameron University

The oxidative stress protein CaSsk1p has been shown to play a role in virulence of Candida albicans, one of the top four causes of nosocomial infectious diseases in humans. The crystal structure of CaSsk1p may help in developing innovative antifungal drugs. This research attempted to clone CaSSK1 gene into an E.coli expression plasmid, in order to tag CaSsk1p with peptides that helps the protein folding during expression.

Bacteria that invade the human body are killed by hypochlorous acid (HOCl) that is generated by the myeloperoxidase system in activated neutrophils. HOCl is considered to be a highly destructive and relatively nonselective oxidant that reacts with a variety of subcellular compounds such as amino acids, peptides, and proteins. The reactions of HOCl with these cellular compounds cause damage to the organism that eventually leads to cell death. It is believed that the respiratory chain of bacteria is a possible target. In this presentation, damage to the respiratory chain caused by the reactions of HOCl has been studied in real time. Bioluminescent E.coli (MG1655lux) that has been transformed with a recombinant plasmid that contains Vibrio fischeri luciferase genes has been used to monitor ATP depletion. In addition, green fluorescence protein (gfp) expressing E.coli (MG1655gfp) are employed to monitor the disruption pH homeostasis in real time.

P18: Experimental Restraints Reduce Folding Space and Enable Computation of a Complete Set of Possible Folding Solutions for a Viral RNA

**Presenter:** Jonathan Stone, Chemistry, U. Oklahoma

**Authors and Affiliation:** S. Schroeder, J. Stone, M. Rowe. University of Oklahoma. Poster to be presented jointly by J. Stone and M. Rowe.

An existing RNA secondary structure prediction algorithm is parallelized and augmented with software filters that enable the enumeration and analysis of a complete RNA secondary structure folding funnel using modern commodity cluster computing hardware. Parallelization and novel software filters addressing experimental knowledge of global structure features including nucleotide solvent accessibility, helix quantity and length, and base pair distance restrictions combine to enable computational access to broader windows into the folding funnel without the need for expensive storage space by filtering structures as they are generated according to user-configurable parameters.
P19: Experimental Restraints Reduce Folding Space and Enable Computation of a Complete Set of Possible Folding Solutions for a Viral RNA

**Presenter:** Montana Rowe, Chemistry/Biochemistry, University of Oklahoma

**Authors and Affiliation:** S. Schroeder, J. Stone, M. Rowe. University of Oklahoma. Poster to be presented jointly by J. Stone and M. Rowe.

An existing RNA secondary structure prediction algorithm is parallelized and augmented with software filters that enable the enumeration and analysis of a complete RNA secondary structure folding funnel using modern commodity cluster computing hardware. Parallelization and novel software filters addressing experimental knowledge of global structure features including nucleotide solvent accessibility, helix quantity and length, and base pair distance restrictions combine to enable computational access to broader windows into the folding funnel without the need for expensive storage space by filtering structures as they are generated according to user-configurable parameters.

P20: Influence of Salivary Defensive Peroxidases on Streptococcal Antagonism in Oral Biofilms

**Presenter:** Michael Ashby, Department of Chemistry and Biochemistry, University of Oklahoma

**Authors and Affiliation:** Michael T. Ashby,1* Jens Kreth,2 Laure S. Sivulu,1 and Muthuvelan Soundarajan1 Department of Chemistry and Biochemistry, University of Oklahoma1 and Department of Microbiology & Immunology, University of Oklahoma Health Sciences2

Oral biofilms are comprised of diverse bacterial species that compete for limited resources. *Streptococcus* is a dominant genus, making up about 20% of the more than 800 species of bacteria that have been identified in the oral cavity, and about 80% of the early biofilm colonizers. Oral streptococci include both health-compatible [e.g., *S. gordonii* (Sm) and *S. sanguinis* (Ss)] and pathogenic strains [e.g., the cariogenic *S. mutans* (*Sm*)]. Because the streptococci have similar metabolic requirements, they have developed defense stratagems that lead to antagonism (a.k.a. bacterial interference). *Sm* expresses bacteriocins that are cytotoxic toward Sg and Ss, whereas Sg and Ss differentially produce H2O2 (under aerobic growth conditions) which is relatively cytotoxic toward Sm. Superimposed on the inter-bacterial combat are the effects of the host defensive mechanisms. This poster focuses on the surprising complex effects of human salivary defensive peroxidases (part of the innate defenses of the oral cavity) on streptococcal antagonism. As expected, we observe no influence of the peroxidase system on the ability of Sm to inhibit the growth of other streptococci vis-à-vis bacteriocins. However, the peroxidase system (comprised of the enzyme and its substrate thiocyanate) destroys H2O2, thereby facilitating the growth of all three streptococci. Apparently, under the conditions of our experiments, the hypothiocyanate (OSCN) that is produced by the peroxidase system is less cytotoxic than the H2O2 that is consumed. Complicating the picture is the fact that the peroxidase proteins themselves inhibit bacterial growth. Thus, a dose-dependent reduction of biomass is observed when cultures are treated with peroxidase (in the absence of thiocyanate). The inhibitory effect of peroxidase protein on biofilm growth of Sm (but not Sg and Ss) is negated in the presence of sucrose. This may be accounted for by the fact that Sm produces more glucans from sucrose, which presumably strengthens the extracellular matrix of its biofilm. The relevance of our finding with respect to human health will be discussed.

P21: Is Cyanogenesis a Virulence Factor of *Pseudomonas Aeruginosa* that Inactivates Human Defensive Peroxidases and their Antimicrobial Hypohalites?

**Presenter:** Michael Ashby, Department of Chemistry and Biochemistry, University of Oklahoma

**Authors and Affiliation:** Michael T. Ashby* and Kelemu Lemma, Department of Chemistry and Biochemistry, University of Oklahoma

*Pseudomonas aeruginosa* (Pa) frequently infects the mucosa of immunocompromised individuals, including the lungs of individuals with cystic fibrosis (CF). The human mucosa of healthy individuals are normally protected by innate defense mechanisms that include peroxidases that produce antimicrobial hypohalites. The lactoperoxidase (LPO) system has been previously recognized to play a pivotal role in controlling the mucosa in general (particularly in saliva, nasal and lachrymal fluids, and breast milk), but its importance in the defense of the airways has only been recently acknowledged. In a physiological setting, the enzyme LPO exclusively catalyzes the oxidation of the pseudohalide thiocyanate (SCN−) by hydrogen peroxide (H2O2) to produce hypohiociyanate (OSCN), as compared to myeloperoxidase and eosinophil peroxidase, which are leukocyte-derived human defensive peroxidases that employ substrates besides SCN−. The LPO system has been shown to eliminate Pa on the airway mucosal surfaces of healthy individuals. Cyanide generally inhibits heme enzymes by coordination to the iron active site. In addition, with the present study we show that OSCN− and CN− react with pH-dependent kinetics to produce SCN− and cyanate (OCN−), with the maximum rate occurring near neutral, physiological pH. Our studies demonstrate that the reaction mechanism involves electrophilic attack of HOSCN of SCN− to give the intermediate dicyanosulfide (NC-S-CN), which subsequently hydrolyzes to yield SCN− and OCN−. In addition to presenting a detailed chemical mechanism for the title reaction, we discuss the possible relevance of cyanogenesis as a virulence strategy by Pa in the CF lung and the possible significance of NC-S-CN and cyanyl radical (CN−).
P22: Mechanism of the Stimulation of MacB ATPase by the Periplasmic Membrane Fusion Protein (MFP) MacA

**Presenter:** Sita Devi Modali, Chemistry and Biochemistry, University of Oklahoma

**Authors and Affiliation:** Sita D. Modali, Helen I. Zgurskaya.

Drug efflux pumps are the main contributors to the failure of antibiotic therapy. In Gram-negative bacteria, these pumps function as tripartite complexes that extrude drugs out of the cells. In *Escherichia coli*, MacA-MacB-TolC is the first experimentally characterized macrolide specific efflux pump. Here, MacB is the ABC type inner membrane transporter, TolC is the outer membrane channel and MacA is the periplasmic Membrane Fusion Protein. MacA physically connects MacB to TolC and also stimulates the ATPase activity of MacB. The C-terminal domain of MacA is essential for the MacB ATPase stimulatory activity. However, the biochemical mechanism of MacA mediated stimulation of MacB ATPase is unknown. In this study, using site directed mutagenesis we identified G353 and G357 residues in MacA which are essential for the stimulation of MacB ATPase *in vitro*. Trypsin proteolysis of the wild type MacA and mutants showed that mutations in these positions affect the conformation of MacA both *in vivo* and *in vitro*. Protein co-purification and proteolytic digests indicate that MacA mutants assemble into the tripartite complex MacAB-TolC. However, mutant complexes are different from those of the wild type MacA. We conclude that the amino acid residues G353 and G357 are essential for the function of MacA in stimulating the activity of MacB ATPase and also for the assembly of the proper MacA-MacB-TolC efflux pump.

P23: Midline-1 has 3 RING fold Domains which all have E3 Ligase Activity

**Presenter:** Xiaofeng Han, Biochemistry And Molecular Biology, Oklahoma State University

**Authors and Affiliation:** Xiaofeng Han, Haijuan Du, Michael A. Massiah* Department of Biochemistry and Molecular Biology, Oklahoma State University, Stillwater, OK, USA 74078.

Midline-1(MID-1) is a microtubule-associated TRIM protein that interacts with alpha-4, a regulatory subunit of the protein phosphatase 2A catalytic (PP2Ac) domain, and targets PP2Ac for ubiquitin-mediated degradation. Mutations of MID1 results in ventral midline malformations in humans, partially due to MID1’s role in the epithelial-to-mesenchymal transformation along the midline. MID1 contains a conserved N-terminal RING, two B-boxes (of type 1 and type 2) and coiled-coil domains and we recently showed that the B-box domains adopted bba-RING folds of domains that have *in vitro* Ub E3 ligase activity. Here we report that MID1 three zinc-binding RING and B-box domains (RF, Bbox1 and Bbox2) possess *in vitro* Ub E3 ligase activity. RF-B1 and RF-B1-B2 show improved *in vitro* Ub E3 ligase activity compared with the individual domains. In targeting PP2Ac for ubiquitination, B-box1 was shown to interact with alpha-4. Here, we show that alpha-4 can also be a target for ubiquitination. Based on these observations, we hypothesized that MID1 three RING folds adopt a novel mechanism for ubiquitinating PP2A for degradation and that there maybe additional target proteins that can be targeted for degradation by MID1.

P24: Prohead RNA Self-Assembly

**Presenter:** Xiaobo Gu, Chemistry and Biochemistry, the University of Oklahoma

**Authors and Affiliation:** Xiaobo Gu, Susan J. Schroeder Department of Chemistry and Biochemistry, University of Oklahoma, 620 Parrington Oval, Norman, OK 73019

Prohead RNA (pRNA) is an essential component of a powerful biomolecular nanomotor that packages bacteriophage genomes into viral capsids. This research presents the thermodynamic stabilities and sequence dependence of tertiary interactions in pRNA self-assembly. The bacteriophage phi29, GA1, M2 and SF5 pRNA self-assemble into dimers, trimers, and multimers in a magnesium ion and temperature dependent manner. The predicted intermolecular Watson-Crick base pairs in the four pRNA sequences vary, but the free energies of self-assembly are all 7-8 kcal/mol. Phi29 pRNA mutants form dimer even if only GU noncanonical base pairs may form. Thus, in addition to the intermolecular base pairs, the tertiary structure around the loops contributes to the energetic stability of the pRNA multimers.


**Presenter:** Koree Clanton Arrowood, Chemistry, University of Oklahoma

**Authors and Affiliation:** Koree Clanton Arrowood, Susan J. Schroeder

Satellite Tobacco Mosaic Virus (STMV) is an ssRNA virus with a genome of 1058 nucleotides that requires tobamoviruses for its replication. The x-ray crystallography structure has been solved for the icosahedral T=1 virus to 1.8Å, showing 30 helices of at least nine base pairs long. Current RNA secondary structure prediction algorithms do not predict structures consistent with the crystallography data. In RNA secondary structure folding algorithms, covariation can be used as an experimental restraint. Site directed mutagenesis is used to look for covariation in the STMV sequence. Traditional random mutagenesis approaches are utilized at the transcriptional level. Varying concentration of Mn $^{2+}$ to Mg $^{2+}$ transcription buffers are
used to cause misinsertions of nucleotides during the transcription with T7 RNA polymerase. This is tested with mutations in restriction enzyme sites in a plasmid. Mutated restriction enzyme sites are no longer cleavable. This same technique is now being used to create STMV mutants used in the search for covarying nucleotides.

8:30 AM - 5:00 PM Ballrooms H and I

Biofuels - Poster

P26: An Efficient Catalytic Deoxygenation Reaction for the Conversion of Biomass-derived Glycols to Alkenes

Presenter: Irshad Ahmad, Chemistry and Biochemistry, The University of Oklahoma

Authors and Affiliation: Irshad Ahmad and Kenneth M. Nicholas*, Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma, OK 73019 Email: knicholas@ou.edu and irshad.ahmad-l@ou.edu

In this study we are seeking new catalytic processes for the deoxygenation of biomass-derived polyols and diols to produce unsaturated alcohols and hydrocarbons of value as chemicals feedstock and fuels. Hence, non-precious oxo-metal complexes Z\textsubscript{1,2}MO\textsubscript{4}\textsuperscript{1,2} (M= Re, Mo, W), an economical thermodynamically-competent reductant Na\textsubscript{2}SO\textsubscript{3} and phase transfer agents were screened for their ability to promote progress towards achieving our goals will be summarized.

\[ \text{RCH(OH)CH}_2\text{OH} + \text{Na}_2\text{SO}_3 \rightarrow \text{RCH=CH}_2 + \text{H}_2\text{O} + \text{Na}_2\text{SO}_4 \]

P27: Anaerobic Biodegradation of Biodiesel and Corrosion

Presenter: Deniz F. Aktas, Botany and Microbiology, University of Oklahoma

Authors and Affiliation: Deniz F. Aktas, Jason S. Lee(2), Brenda J. Little(2), Irene A. Davidova(1), Christopher N. Lyles(1) and Joseph M. Suflita(1), Department of Botany and Microbiology and Institute for Energy and the Environment, University of Oklahoma, 770 Van Vleet Oval, Norman, Oklahoma 73019 (2)Naval Research Laboratory, Stennis Space Center, MS 39529

Biodiesel is composed of monoaalkyl esters of long chain fatty acids derived from renewable lipid sources. Despite the global acceptance of biodiesel, the full impact of integrating biodiesel with the existing infrastructure has not been fully explored. The biodiesel susceptibility to biological attack in the absence of oxygen is examined by incubating five different marine and freshwater anaerobic inocula in biodiesel amended incubations, which indicated the direct link between biodegradation and corrosion. Gas chromatography/mass spectrometry revealed that the methyl esters of biodiesel were readily hydrolyzed by the various inocula and a complex but similar suite of fatty acids was found as metabolic intermediates. This study showed that biodiesel can be rapidly biodegraded under anaerobic conditions. We will summarize our findings on the metabolic intermediates, reaction conditions, preliminary results and a suggested mechanism of this novel conversion will be presented.

P28: Catalytic Conversion of Diols to Alkenes via Epoxide

Presenter: A.K. Fazlur Rahman, Chemistry, Oklahoma School of Science and Mathematics

Authors and Affiliation: A.K. Fazlur Rahman, Department of Chemistry, Oklahoma School of Science and Mathematics, 1141 North Lincoln Blvd, Oklahoma City, OK 73104 And Kenneth M Nicholas, Department of Chemistry University of Oklahoma, Norman, OK 73104

We employed metal carbonyl cations as Lewis acid to catalyze the dehydration of diols to epoxide. The epoxide is then converted to alkene by using carbon monoxide as a reducing agent. Specific examples of metal carbonyl cations, reaction conditions, preliminary results and a suggested mechanism of this novel conversion will be presented.

P29: Methyltrioxorhenium Catalyzed Deoxygenation of Glycols and Epoxides to Alkenes utilizing Sodium Sulfite as a Reductant

Presenter: Garry Chapman Jr., Chemistry and Biochemistry, University of Oklahoma

Authors and Affiliation: Garry Chapman Jr. and Dr. Kenneth Nicholas*, Department of Chemistry and Biochemistry University of Oklahoma, Norman, OK 73019 Email: garrychapman@ou.edu

We are currently exploring new catalytic methodology for the deoxygenation of bio-mass derived glycols and epoxides, in an effort to produce valuable unsaturated hydrocarbons. Our current catalytic system for such purpose employs the oxo-metal complex catalyst methyltrioxorhenium (MOTOR) and utilizes the economical and effective reductant sodium sulfite (Na\textsubscript{2}SO\textsubscript{3}) (eq 1). We will summarize our findings on the MOTOR – catalyzed reactions showing that moderate yields of alkenes are obtained from glycols and epoxides.

\[ \text{R-CH(OH)CH}_2\text{OH} + \text{Na}_2\text{SO}_3 \rightarrow \text{R-CHCH}_2 + \text{Na}_2\text{SO}_4 + \text{H}_2\text{O} \]
Enzymatic biofuel cells represent an important alternative to batteries and conventional fuel cells as they are able to produce electricity under mild conditions and with renewable catalysts and fuels. Their potential applications include the replacement of batteries in small electronic devices, and implantable electrical devices such as pacemakers and glucose meters. For most biofuel cell electrodes, enzymes are immobilized on the surface of an electrode along with an electrochemical mediator. The mediator can be any number of redox-active species, including osmium, quinone compounds, and ferrocene. Recently, our group developed a series of unique redox polymers based on ferrocene-modified linear poly(ethyleneimine) (LPEI) which, when cross-linked in the presence of glucose oxidase, display high sensitivity and current densities of ~1 mA/cm² as glucose linked in the presence of glucose oxidase, display high linear poly(ethylenimine) (LPEI) which, when cross-linked unique redox polymers based on ferrocene-modified recent studies show that we can furnish this choice merely by substituting the metal chloride for FeCl₃ in the synthesis. Dinitrosyl iron complexes have been invoked as viable entities that contribute towards the biological action of nitric oxide (NO). Synthetic iron dinitrosyl compounds display a variety of properties including the ability to transfer molecular oxygen to phosphines or alkenes, and the ability to serve as catalysts for the dimerization of olefins. Thus, the development of advanced undergraduate laboratory experiments in this field is both timely and appropriate. We have developed a prototype undergraduate research project involving the preparation of a series of dinitrosyl iron complexes of the form Fe(NO)₂L₂ (L = phosphine donor ligand). Preparing and characterizing these types of derivatives will provide students with the opportunity to learn and utilize a number of advanced laboratory techniques including the manipulation of air sensitive compounds, infrared and NMR spectroscopy, electrochemistry and infrared fiber-optic spectroelectrochemistry. This work was supported in part by a United States Department of Education GAANN fellowship.

P31: Metal-Oxalate Complex Salts: Teaching an Old Lab New Tricks
Presenter: Stephen Prilliman, Chemistry, Oklahoma City University
Authors and Affiliation: Kayla Smithhart, Oklahoma City University, Oklahoma City, OK

The synthesis of potassium ferrioxalate hydrate, K₃[Fe(C₂O₄)₃]·3H₂O, is a common inorganic synthesis and analysis experiment in General Chemistry Lab. This lab is popular because the synthesis product can be analyzed using titrations, gravimetric analysis and/or absorption spectroscopy to determine the percent composition and empirical formula of the compound. However, the lab is very “cook-book” and can become tedious for both students and instructors. In this work we are allowed students to vary the metal cation center from Fe²⁺ to Cu²⁺, Co²⁺, Al³⁺, Fe³⁺, and Ni²⁺. Students would be allowed to choose their metal ion center, complete the synthesis and pool their results with their classmates. This allows students to see the wide variety of complex ion salts and analyze their similarities and differences. Preliminary results show that we can furnish this choice merely by substituting the metal chloride for FeCl₃ in the synthesis.
tomato paste and the extraction techniques. These inconsistencies led to confusing experimental results that did not effectively instruct the students on column chromatography. Seeking a solution for this problem, the authors began researching other experiments which could teach chromatic techniques and provide an open-ended result from the students prospective. The presenter will discuss the experiments that were evaluated and the process for developing the open-ended experiment, Isolation and Identification of Anthraquinone Dyes, that will be introduced to the Organic Chemistry Laboratory curriculum this summer.

P34: The Spectroscopy of Stars and Applications for Students
Presenter: Stephen Prilliman, Chemistry, Oklahoma City University
Authors and Affiliation: Christopher Ayres Oklahoma City University, Oklahoma City, OK

This project introduces students to a genuine application of spectroscopy in a laboratory setting, obtaining and analyzing the spectra of night-time stars. The spectrometer is a published design utilizing simple classroom materials such as cardstock, a DVD, and tape. Other materials needed are an amateur telescope and a digital camera. From these materials, and making slight alterations to the published design to fit our camera and telescope, we hope to obtain spectral blackbody profiles and atomic line spectra from stars.

8:30 AM - 5:00 PM Ballrooms H and I
Environmental Chemistry - Poster

P35: A Model of Anaerobic Oxidation of Methane via the Fumarate Addition Mechanism Using DFT Calculations
Presenter: Keisha Beasley, CEES, University of Oklahoma
Authors and Affiliation: Keisha K. Beasley and Mark A. Nanny School of Civil Engineering and Environmental Science, University of Oklahoma, Norman, Oklahoma 73019

Microbially mediated anaerobic oxidation of methane is considered an important sink for dissolved methane in open ocean water and some surface water. The mechanism and microbial communities responsible for this oxidation are not fully known. Using quantum chemical calculations, fumarate addition to methane is examined as a thermodynamically feasible mechanism for biological attenuation of methane. The objective of this study is to create a reaction coordinate to determine if the reaction is thermodynamically viable, and to provide information about the energetic barriers of the reaction to compare to those of more readily transformed substrates. A reaction coordinate for the proposed fumarate addition reaction for methane is generated using the uB3LYP/6-31+G(d,p) exchange-correlation functional and basis set. The results suggest the reaction is thermodynamically plausible with a calculated overall free energy change of approximately -34 kcal/mol and the hydrogen atom abstraction from methane is calculated to be the rate-limiting step (approximate Ea = 17 kcal/mol). This suggests that fumarate addition to methane could be responsible for the attenuation of dissolved methane in natural waters. A comparison of activation energies indicated that the energy required for the initial hydrogen atom abstraction may dictate the degree to which hydrocarbons are biodegraded in the environment.

P36: Comparison of Methyl Glucamine and Glycoside Surfactant Headgroup Synergism with Alkyl Carboxylic Acid Salts
Presenter: Louis Jackson, Engineering, University of Oklahoma
Authors and Affiliation: Dr. Brian P. Grady, Demarco Jones

Currently, surfactant containing detergents and cleaning products are discharged into wastewater which can result in toxic effects on microbial and aquatic populations. Synergetic interactions between different types of surfactants may result in lower detergent usage and emission. Further, the use of surfactants derived from petroleum-based sources is thought to be not as environmentally friendly as those from renewable resources; this study uses surfactants from renewable resources. In this study, mixtures of alkyl N-methyl glucamines with linear alkyl carboxylic acid salts and alkyl glucopyranosides (glycosides) with linear alkyl carboxylic acid salts are currently being investigated. Solutions at various concentrations and mixture ratios were tested and evaluated to determine critical micelle concentration (CMC), surface tension at the CMC, and surface tension reduction efficiency. In previous investigation of alkyl sulfates, a much greater interaction was seen between the sulfate headgroup and the methyl glucamine headgroup which was attributed to the more flexible nature of the glucamine headgroup relative to that of the glycoside headgroup. Similar synergistic trends of alkyl carboxylic acid salts/alkyl methyl glucamine vs. alkyl carboxylic acid salts/alkyl glycoside are expected here, and this poster will present the results to this point of that study.
P37: Bio-Coordination Chemistry: Transition Metal CXCR4 Antagonists

Presenter: Tim Hubin, Chemistry, Southwestern Oklahoma State University

Authors and Affiliation: Timothy J. Hubin,1 Amy N. Cain,1 Orry C. Birdsong,1 Kimberly D. Roewe,1 Courtney D. Garcia,1 Desiray J. Cannon,1 Stephen J. Archibald,2 Graeme McRobbie,2 Abid Khan,2 Christophe Pannecouque,3 Erik DeClercq,3 Tony Ng4 1) Southwestern Oklahoma State University, 2) University of Hull, United Kingdom, 3) Rega Institute for Medical Research, Katholieke Universiteit Leuven, Belgium and 4) King's College London

Objectives: The CXCR4 co-receptor is a known entry route for HIV into cells, generating interest in a therapeutic approach to treatment via fusion inhibitor drugs. A bis-tetraazamacrocycle compound, AMD3100, has been studied intensively as a potential CXCR4 antagonist. Our aim is to develop new antagonists for the CXCR4 co-receptor. They are conformationally fixed bis-macrocyclic transition metal complexes inspired by AMD3100.

Methods: Bis-tetraazamacrocycle ligands conformationally fixed by the addition of two-carbon bridges have been designed and synthesized, along with their Cu2+, Ni2+, Cu2+ and Zn2+ complexes. X-ray crystallography has revealed the complex conformations. Anti-HIV activity screening and CXCR4 binding studies have been performed.

Results: X-ray crystallography has shown the expected conformational selectivity of the complexes. Anti-HIV screening has revealed these complexes as highly active fusion inhibitors. CXCR4 binding studies have shown strong binding of the complexes in competition with CXCR4-specific monoclonal antibodies.

Conclusions: Conformational fixing of the ligand system has resulted in enhanced residence time of these antagonists relative to AMD3100. This result likely explains the efficient antagonism of CXCR4 by these complexes.

Funding was provided by Research Corporation CC6505 (TJH); NIH Grant P20 RR016478 (TJH); Yorkshire Cancer Research YBC157 (SJA); Yorkshire Concept Fund EBC012 (SJA)

P38: Hydroxamate Iron Porphyrinates as New Synthetic Model for the Active Site of Catalase

Presenter: Adam Warhausen, Chemistry and Biochemistry, University of Oklahoma

Authors and Affiliation: Adam Warhausen, Douglas R. Powell, and George B. Richter-Addo, Department of Chemistry and Biochemistry, University of Oklahoma, 620 Parrington Oval, Norman, OK 73019

Catalase is an important enzyme that is responsible for the destruction of hydrogen peroxide in cells. The active site of the enzyme contains a heme-alkoxide functionality of the form (por)Fe(OR); however, the tyrosinate proximal ligand is stabilized by a hydrogen bond system. The development of active site models for catalase remains a priority in bioinorganic chemistry. Hydroxamic acids are utilized in nature for a variety of functions including metal chelation. Hydroxamic acids coordinate to metals typically in a bidentate fashion, although we have shown coordination to iron porphyrins is usually in a monodentate fashion. In this current study, we have prepared new iron porphyrin alkoxide compounds of the form (por)Fe(OR) (where OR is the alkoxide). The alkoxides we chose for this study contain a hydroxamate function group that does not bind to the heme iron. In this way, we generate an internal hydrogen-bond stabilization of the bound alkoxide ligand. Our results on the preparation, spectral characterization, electrochemistry, and single-crystal crystallography on a representative new catalase model will be presented and discussed.

P39: Improved Synthesis of Sodium Molybdenum Bronze

Presenter: Cory Perkins, Chemistry, Oklahoma State University

Authors and Affiliation: Cory K. Perkins, Kevin N. Barber, and Allen W. Apblett

The most commonly used synthetic method for production of sodium molybdenum bronzes, originally developed by Thomas and McCarron, is extremely wasteful since it uses large amounts of sodium molybdate as a buffer. This study examines several more efficient (greener) methods for the synthesis of the sodium product including an optimized molybdate-buffered reaction and the use of alternative buffers such as bicarbonate. The bronze products thus produced were subsequently characterized in terms of sodium content, the number of reducing equivalents, and the degree of hydration. One application of the sodium bronze material as a fast response, chemiresistive peroxide vapor detector will also be highlighted.
P40: Organoruthenium Porphyrins With O-Bound Ligands Trans To Nitric Oxide
Presenter: Dennis Awasabisah, Chemistry and Biochemistry, University of Oklahoma
Authors and Affiliation: Dennis Awasabisah, Nan Xu, George B. Richter-Addo University of Oklahoma

Iron porphyrins have established biological chemistry dependent on the metal center’s reactivity. In addition, nitric oxide (NO) is a biologically relevant signaling molecule that binds to Fe porphyrins as part of its biological function. Ruthenium is commonly used as a model for Fe because of the increased strength of Ru-ligand bonds. We have prepared Ru porphyrins with NO as an axial ligand from the reaction of (por)Ru(CO) precursors with alkyl nitrites. The resulting (por)Ru(NO)(OR) complexes have been isolated and characterized by IR and NMR spectroscopy. These compounds are moderately stable in air as solids, but are found to be reactive with carboxylic acids in solution. For example, the reaction of a typical (por)Ru(NO)(OR) complex with the carboxylic acid R'C(=O)OH generates the (por)Ru(NO)(OC(=O)R') derivative in good yields. The preparation, characterization, and reaction chemistry of these complexes will be presented and discussed.

P41: Structural Investigations into the Heme Nitrosamine Interaction
Presenter: Nan Xu, Chemistry and Biochemistry, University of Oklahoma
Authors and Affiliation: Douglas R. Powell, George B. Richter-Addo University of Oklahoma

Nitrosamines belong to the general class of N-nitroso compounds, and are generally considered to be carcinogenic. However, they require metabolic activation by the cytochrome P450 enzymes via interaction with their heme active sites. Nitrosamines can bind to the protein distal pocket amino acids (Type I interaction) or can bind directly to the ferric Fe centers. Despite the vast knowledge available on the P450-induced metabolism of carcinogenic nitrosamines, there was no information on the structures of these proposed heme-nitrosamine adducts prior to our work in this area. We have prepared and characterized, by spectroscopy and crystallography, a series of thermally stable ferric heme-nitrosamine complexes. We show that the nitrosamines bind to the ferric centers via the O-binding mode. The structural consequences of such O-binding on the metabolic chemistry will be presented and discussed.

P42: Synthesis and Biological Studies of Nicotinic Acid and Thionicotinic Acid Metal Complexes
Presenter: A.K. Fazlur Rahman, Chemistry, Oklahoma School of Science and Mathematics
Authors and Affiliation: Margaret Wang, Tara Sarathi, Lisa Zhang and A.K. Fazlur Rahman Department of Chemistry, Oklahoma School of Science and Mathematics 1141 North Lincoln Blvd, Oklahoma City, OK 73104 and Doug Powell Department of Chemistry University of Oklahoma, Norman, OK 73019

Niacin, also called nicotinic acid or water soluble B3, is commonly synthesized in human body in a two step enzyme catalyzed conversion. In this project we have synthesized 2-mercapto nicotinic acid and 2-mercapto salicylic acid complexes of copper and manganese. In the case of copper the 2-mercapto nicotinic acid formed a dimeric compound. Crystal structure analysis shows that during the course of the reaction the RSH group has converted to RSO2H group. The redox chemistry of this process along with the crystal structure and biological activity will be discussed during the presentation.

P43: Capillary electrophoresis separations of nanoparticles
Presenter: Thushara Athauda, Chemistry and Biochemistry, University Of Tulsa
Authors and Affiliation: Thushara Athauda, Slawomir Oszwaldowski, Brian Walker, and Kenneth P. Roberts Department of Chemistry and Biochemistry, University of Tulsa, 800 S.Tucker Dr., Tulsa, Oklahoma 74104

Capillary electrophoresis (CE) was used for the characterization of water-soluble CdSe/ZnS quantum dots (QDs) and their conjugates to chemical and biochemical surface ligands. We found that QD conjugates were efficiently separated from free QDs by optimization of typical CE separation parameters. The surface-modified QDs were also characterized by UV-VIS and photo-luminescence spectrophotometry, gel electrophoresis, dynamic light scattering, TEM and surface charge (zeta potential) measurements. It is believed that these results will aid in the further development of nanoparticles in chemical and biochemical assays and devices.
P44: Characterization of Multiwalled carbon nanotube polymer composites
Presenter: Robert Headrick, Research and Development, SouthWest Nano Technologies
Authors and Affiliation: Robert Headrick, Yongqiang Tan, Ricardo Prada Silvy, Dave Arthur, (SWeNT) Brian P. Grady, (OU) Petra Pötschke (Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden, Germany)

To compare and optimize the multi walled carbon nanotubes polycarbonate composite, carbon nanotubes from different sources were melt mixed at seven different concentrations into the polymer matrices. Characterization of electrical conductivity was investigated by gluing copper probes with a silver epoxy to the surface of the polymer then applying a voltage and measuring the current. This data was then analyzed to produce resistivity measurements per type of carbon nanotube. A Differential Scanning Calorimeter was used to identify any changes in the glass transition temperature of the polycarbonate. Each sample was tested upon cooling at 1 C/min from 200C to 100C. Scanning electron microscopy was used to provide visuals of the carbon nanotube dispersion throughout the matrices. Future analysis will include tensile testing to identify each composite’s modulus of elasticity. Also, dynamic mechanical analysis will contribute to the data by tension and three point bend testing.

P45: Controlled growth and differentiation of mesenchymal stem cells on bacteriophage films
Presenter: Haibao Zhu, Chemistry And Biochemistry Department, The University Of Oklahoma
Authors and Affiliation: Haibao Zhu, Binrui Cao, Chuanbin Mao Chemistry And Biochemistry Department The University Of Oklahoma

To investigation of growing mesenchymal stem cells (MSCs) on the M13 phage matrices demonstrated that the phages were able to maintain cell viability, proliferation, and differentiation. We employed a 2D substrate coated with M13 phage nanofiber. M13 phage nanofiber is approximately 6.5 nm in diameter and 880 nm in length. It has been used in human medical trials as tumor-targeting vehicles and in animal studies for targeted delivery of drugs and imaging agents. The temporal effect of phage coated substrate on the morphology, proliferation and differentiation capacity of the MSCs was assayed. The morphology of MSC growth on the phage film generated by different concentrations of phage was different. The phage films directed MSCs along a predictable direction and the cells were found to be elongated.

P46: Development and characterization of fast-acting microspheres for thrombolytic therapy
Presenter: Hoai Nguyen, Chemical, Biological & Materials Engineering, University of Oklahoma
Authors and Affiliation: Hoai Nguyen,1 Edgar O’Rear,1 Eugene Patterson2 1. School of Chemical, Biological and Materials Engineering, University of Oklahoma Bioengineering Center, 2. Department of Cell Biology, University of Oklahoma Health Sciences Center
Microspheres for fast-acting purpose in thrombolytic therapy are being developed so that their action should be slightly delayed. A polymer that allows the release of an active agent within minutes or hours is required for this application. Eudragit S100 is an anionic polymer synthesized from methacrylic acid and methyl methacrylate and has a pH-dependent solubility. It is slowly soluble in the medium of pH>7. Eudragit S100 and bovine serum albumin (BSA) are used as polymer and model protein for the preparation of microspheres by the double emulsion method. In this study, microspheres were characterized by their morphology, particle size, encapsulation efficiency and release profile of BSA in vitro. Influence of the preparation conditions on the particle size, encapsulation efficiency, and release profile in vitro was investigated.

P47: Effect of Single-Walled Carbon Nanotube Association upon Representative Organonitrogen Compounds
Presenter: Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma
Authors and Affiliation: Donna J. Nelson,* Panneer Selvam Nagarajan, and Christopher N. Brammer, Department of Chemistry, University of Oklahoma, Norman, OK djnelson@ou.edu

Some organic solvents facilitate single-walled carbon nanotube (SWCNT) dispersion via association. Nuclear magnetic resonance (NMR) was previously used to probe causative interactions in SWCNT:amide associations by determining the influences of SWCNTs upon 1H NMR spectra of amides, which have adjacent nitrogen and oxygen functionalities. Those studies are now extended to SWCNT associations with aminocarbonyls, aminooalcohols, and an oxime in order to explore effects upon these interactions due to (A) cyclization, (B) separating functionalities by one or more carbons, and (C) using different nitrogen and oxygen functionalities. The change in 1H NMR chemical shift magnitude and shape of the signal represents the strength and type of the association with SWCNTs: (1) Both cyclization and nitrogen-oxygen proximity influence the association, (2) SWCNT association with nitrogen lone pairs is stronger than with those of oxygen, (3) proton proximity to nitrogen or oxygen increases effects of association with SWCNTs, and (4) protons bonded to heteroatoms are influenced more than protons bonded to carbon.
**P48: Effects of Sodium Bicarbonate Treatment on the Structure of Single Walled Carbon Nanotube Brands Studied by Raman and Ultraviolet-Visible Spectroscopy**  
**Presenter:** Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma  
**Authors and Affiliation:** Donna J. Nelson, Murali Murugesan, and Christopher N. Brammer Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK 73019, USA djnelson@ou.edu

Single walled carbon nanotubes (SWCNTs) in polymer blends enhance properties more greatly and consistently if the SWCNTs used are pure. However, the impurities in SWCNT samples “as received” are often not known, the manufacturer's purity statements not verified, and purification techniques not compared or standardized. The effects of sodium bicarbonate (NaHCO₃)treatment and oven drying on the level of impurities in three brands of single walled carbon nanotubes-SWCNTs (SWeNT, HiPco and NanoLab) are studied using Raman spectroscopy and ultraviolet-visible spectroscopy (UV-Vis). The removal of impurities from “as received” p-SWCNT by NaHCO₃ washing and oven drying was evidenced from an improvement in UV-Vis spectra of the purified SWCNTs. Change in the Raman G/D ratio of “as received” p-SWCNTs by NaHCO₃ washing and oven-drying also supports the UV-Vis results. The presented p-SWCNT purification methods and consistent characterization support the current effort to develop purity evaluation criteria and quality assurance standards for carbon nanotubes, while moving from a strong acid or base purification, to a mild environmentally-friendly technique.

**P48: Effects of Sodium Bicarbonate Treatment on the Structure of Single Walled Carbon Nanotube Brands Studied by Raman and Ultraviolet-Visible Spectroscopy**  
**Presenter:** Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma  
**Authors and Affiliation:** Donna J. Nelson, Murali Murugesan, and Christopher N. Brammer Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK 73019, USA djnelson@ou.edu

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**P49: Emulsion Systems Stabilized And Catalyzed By Janus-Silica-Nanoparticles-Supported Catalysts**  
**Presenter:** Maria Ruiz, CBME, University of Oklahoma  
**Authors and Affiliation:** M. Pilar Ruiz, Jimmy Faria and Daniel E. Resasco School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, Oklahoma 73019

Recently, it has been seen that nanohybrids composed of carbon nanotubes fused to oxide particles can be used to stabilize emulsions and, after the deposition of the active metal, catalyze reactions at the water/oil interface[1,2]. In this context, another type of particles that could have the same behavior as the nanohybrids, are the so-called Janus particles. The amphiphilic character of the Janus particles makes them suitable for the stabilization of emulsions[3], besides they can be used as support in catalysts.

In this work, we have synthesized catalysts supported on Janus silica-nanoparticles in order to catalyze reactions at the water/oil interface in biphasic systems. The main goal is to deposit the active metal either simultaneously on the entire surface of the Janus particles, or selectively on the hydrophobic or hydrophilic side. In this way, we can have a total control for directing reactivity in one of the phases, with all the advantages that this achievement implies.


**P50: Evaluation Of Liposome Encapsulated Hemoglobin In Hemorrhagic Shock By Mr Spectroscopy**  
**Presenter:** Hrushikesh Agashe, Pharmaceutical Sciences, College of Pharmacy  
**Authors and Affiliation:** Hrushikesh Agashe, Pallavi Lagisetty, Vibhudduta Awasthi College of Pharmacy, OUHSC, Oklahoma City

While severe hemorrhage is responsible for approximately 3 million deaths worldwide, inadequate and unreliable availability of whole blood or red blood cells still remain a problem. Nanometer-sized liposome-encapsulated hemoglobin (LEH) closely mimics the oxygen carriage, diffusivity and delivery of the RBCs, and is believed to have better control over hemodynamics compared to modified hemoglobin products.

LEH of size 250 nm was manufactured using high-pressure homogenization. The encapsulation of hemoglobin was enhanced by incorporating a novel synthetic anionic lipid, CHHDA, in the phospholipid bilayer. The LEH was characterized for oxygen affinity, size, hemoglobin, methemoglobin, and phospholipid concentration. The resuscitation performance of LEH was evaluated in a rat model of 40% hemorrhagic shock. We monitored cerebral tissue energetics with magnetic resonance spectroscopy (MRS). Mean arterial pressure and hematocrit were monitored throughout the study.

The MRS results demonstrated the potential of LEH as a hemoglobin-based oxygen carrier for use in resuscitation after acute blood loss.
P51: Fluorescence and Raman Spectroscopy of Carbon Nanotubes
Presenter: Chase Brown, Lab, Southwest Nanotechnologies
Authors and Affiliation: Southwest Nanotechnologies

Carbon nanotubes reveal their remarkable structural properties in Raman and UV-Vis spectroscopy. The certain wavelengths they absorb can tell us about the distribution of certain types of arrangements of nanotubes are within the sample. Our preparation of single wall nanotubes is achieved by an hour of sonication in a sodium cholate surfactant to suspend the nanotubes, followed by centrifuging to remove any remaining bundles. This solution is then submitted for analysis to find properties such as amount of metallic and semiconducting nanotubes, diameter, and chirality.

P52: Formation of Hydrophobic Thin Film on Cotton by Admicellar Polymerization
Presenter: Pratik Kothary, Department of Chemical Engineering, University of Oklahoma
Authors and Affiliation: Pratik Kothary, Srinivas Hanumansetty and E.A. O’Rear Chemical, Biological and Materials Engineering, University of Oklahoma, Norman 73019, USA

Admicellar polymerization has been used to modify surfaces of natural and synthetic fibers. The method allows selection of components to yield fabrics with a wide variety of added properties such as water repellency, antimicrobial capability, electrical conductivity, and protection from UV radiation. We have used the process to coat thin film on cotton, to impart hydrophobic character. Processing involves surfactant-facilitated adsorption of monomer on fabric surface followed by polymerization, forming a thin film of fluoropolymer on the surface. Surfactant-monomer systems of fluoronomomers and different classes of surfactants were used. Parameters such as concentrations of surfactant and monomer, and the fabric to liquid ratio were varied for the systems. Results show that hydrophobic thin films can be formed over a wide range of fabric to liquid ratios, and concentration of monomers.

The quality of the thin film has been evaluated by gauging hydrophobic character of the fabric; by observing uniformity of the film and by imaging with SEM.

P53: Improved Electrical Conductivities Of SWNT/Silica Hybrid And UHMWPE Composites Prepared By Sintering Method
Presenter: Cristina Caamaño, Chemical, Biological and Materials Engineering, University of Oklahoma
Authors and Affiliation: Cristina Caamaño, Daniel Smith, Bryan Grady and Daniel E. Resasco

A new cost-competitive single-walled carbon nanotube SWNT/silica hybrid was used as a filler to produce composites in a polymer matrix of ultra high molecular weight polyethylene (UHMWPE). Three different hybrids were used as well as a purified hybrid filler for comparison. Composites were prepared without any functionalization of the fillers by a dry-mixing method, followed by a sintering, which is a compression molding process of dry blends. A segregated network was obtained from the sintering method. Regular melt processing methods does not work well for the UHMPE due to its high melt viscosity and to show that, we also prepared composites by the extrusion method. In this segregated network, a significant dispersing role of the silica was observed, which leads a low percolation threshold of 0.23 wt% for the SWNT/silica hybrid with larger silica content and longer SWNTs. Higher values of 3.8% were found using purified SWNT and no percolation threshold was noticed in extruded SWNT/silica hybrid composites. An important fact is that each composite was made without any dispersion method of the filler in the polymer matrix. Raman spectroscopy is a useful tool to measure dispersion on thin cross sections of composites; we found better dispersion in the composites with hybrids than in the composites with purified SWNT. Significant increases in stiffness were found for composites with hybrids, however, the tensile strength and the elongation at break decreases as the SWNT content increases. DMA frequency and temperatures sweeps show an increase in storage modulus as the hybrid composition increases. DSC non-isothermal analysis shows no change in the crystallization exothermic curves demonstrating the non-nucleation agent effect of these SWNT/silica hybrids, furthermore, the fractional crystallinity decreases 10% between 0% to 0.7% wt% of SWNT in the SWNT/silica hybrid composites.

P54: Influence of the Silica Catalyst Support on the Chirality Distribution of Single Wall Carbon Nanotubes
Presenter: Tyler Ledlow, University of Oklahoma
Authors and Affiliation: Tyler Ledlow, Ricardo Prada, Silvy, Yongqiang Tan, Dave Arthur SouthWest NanoTechnologies, 2501 Technology Place, Norman, Oklahoma, 73071

The influence of the surface area of the silica catalyst support on the carbon nanotube chirality distribution was investigated. Commercial silicas having specific surface areas between 130 m²/g to 400 m²/g were employed. Cobalt molybdenum catalysts were prepared by impregnation of the silica supports with a metallic solution followed by drying and calcination steps at 450 C. Carbon nanotube synthesis was conducted at 700 C in the presence of CO flow using a fluidized bed reactor (CoMoCAT process). Both the product obtained after the reaction and the purified single wall carbon nanotube material obtained from the different catalysts were characterized by Optical Absorption (OA), Raman Spectroscopy, Scanning Electron Microscopy (SEM) and Thermo-Gravimetric Analysis (TGA) techniques. The
results indicate that the surface area modifies the particle size distributions of the metallic cobalt aggregates, therefore defining the chirality distribution of the carbon nanotubes. High surface area of silica support increases the selectivity to 6.5 chirality while lower surface area increases the selectivity to 7.6 chirality. These semiconducting SWCNT hold promise for enabling new generation of sensors and flexible electronics based on inexpensive printed, thin-film transistors.

P55: Known and Predictable MWNT Structure by Adjusting Metal-Support Interactions in Active Catalysts

**Presenter:** Veronica Irurzun, CBME, University Of Oklahoma

**Authors and Affiliation:** Veronica M. Irurzun, Rolf E. Jentoft, James E. Brown III, Ricardo Prada, Daniel E. Resasco*

The production of carbon nanotubes (CNT) with known and predictable structure has become an important area in the nanotubes field since there are multiple applications in which they could be used [1-3]. Among the production techniques, chemical vapor deposition (CVD) is not only the least expensive but also the easiest to scale up to be used in industry. In several of our previous studies [4-7] we have shown that the structure of single-walled carbon nanotubes (SWNT) can be controlled by varying different conditions either related to the catalyst or to the reaction. However, there are a number of important applications that are more suited for multi-walled carbon nanotubes (MWNT). Therefore, it is important to develop similar degree of control in MWNT growth as that reached with SWNT. In this study, we have investigated the effects of varying in a controlled way the interactions between the active metals and the supports on the resulting CNT morphologies. It is shown that characteristics such as number of walls, diameter, and length, can be changed in a systematic fashion by varying parameters related to the catalyst synthesis and the reaction conditions [8-11].

Explosives pose a deadly risk to our society as a consequence of intentional use by terrorists and accidental detonation resulting from mishandling of explosives, discharge of unexploded ordnance, or even build up of peroxides in otherwise safe solvents such as in the everyday lab. We have developed solutions of Microcrystalline Hydrogen Bronzes that are formed from the trioxides of (MoO₃) by the incorporation of hydrogen between the sheets of MoO₃. Our research has shown that when these materials are exposed to a strong oxidizing agent such as H₂O₂, the material will demonstrate colorimetric effects. The nanomaterial will also neutralize the effect of an explosive material such as triacetonetriperoxidediamine(TATP) or hexamethylenetriperoxidediamine(HMTD). These nanomaterial’s with the above effects could serve as potentially useful agents for bomb squads, the military, airports, or even in laboratories where build up of peroxides could be potentially be dangerous. These are just a few entities that might be interested in our research.

The effect of the weight fraction of multi-walled carbon nanotubes (MWCNTs) in high-density polyethylene (HDPE) / MWCNTs composites on their conductivity behavior, crystallinity and mechanical properties is presented here. Samples from a masterbatch consisting of 20.23 wt. % MWCNTs in HDPE were mixed in a DSM micro-compounder with varying amounts of neat HDPE to form composite mixtures of different MWCNT compositions ranging from 1 to 10 wt. %. These samples were compression molded into sheets using high pressure and temperature for analysis. Conductivity measurements showed that percolation occurs at approximately 4 wt. % MWCNTs. Filler incorporation had mixed effects; while the modulus increased with MWCNTs concentration, the overall effect on the tensile strength was much less evident. The elongation at break dropped significantly with filler incorporation. The addition of multi-walled carbon nanotubes also reduced the fractional crystallinity of the polymer matrix measured with wide-angle X-ray scattering (WAXS) and differential scanning calorimetry (DSC). Non-isothermal crystallization measurements indicated that the MWCNTs did not nucleate crystallization for this system.

The photocatalytic activity and the reactivity of SrTiO₃ doped with chromium and co-doped with antimony and chromium have been studied for acetaldehyde adsorption and the photooxidation reaction using FT-IR spectroscopy. Doped metals increase the efficiency as a semiconductor. On both Cr doped and Cr, Sb doped SrTiO₃, acetaldehyde can react to produce crotonaldehyde via the aldol condensation. In the photooxidation, the antimony and chromium co-doped SrTiO₃ showed the higher rate of decomposition of acetaldehyde. The reason of the high photocatalytic activity may be that antimony and chromium stabilize the charge balance by suppression of Cr⁶⁺ ion on the surface.

Two different methods of surface modification of cotton fabrics are compared: direct fluorination using elemental fluorine and admicellar polymerization which uses a surfactant and fluoronomomer system. Sample characterization includes Infrared spectroscopy, analysis of mechanical properties, analysis of wetting times, contact angle measurements, scanning electron microscopy, elemental analysis and atomic force microscopy analysis. Fourier transform infrared spectroscopy and elemental analysis showed the presence of fluorine moieties. In all cases, the presence of very thin polymeric layer on the surface was confirmed, but differences in terms of amount of polymer formed, surface chemistry was found.
P61: Silica encapsulation of Luminescent CdSe/ZnS Nanoparticles
Presenter: Naga Koduri, Chemistry and Biochemistry, University of Tulsa
Authors and Affiliation: Naga Koduri, Kathryn Swenson, Laura Gribbsy, and Kenneth P. Roberts Department of Chemistry and Biochemistry, University of Tulsa, 800 S.Tucker Dr., Tulsa, Oklahoma 74104

Luminescent semiconductor nanocrystals, commonly known quantum dots (QDs), have been given much attention for a wide range of potential chemical and biological applications. However, the cytotoxicity of QDs complicates some biochemical assays and requires special disposal considerations. Therefore, we have developed a method for encapsulating QDs in a functional silica matrix. Encapsulation was facilitated by use of an oil-in-water microemulsion to control the monodispersity and silica shell thickness. It is anticipated that the silica encapsulation will reduce the toxicity of QDs as well as preserve the luminescence properties of QDs.

8:30 AM - 5:00 PM Ballrooms H and I
NMR - Poster
P62: Glass Transitions, Segmental Dynamics, and Friction Coefficients for Individual Polymers in Multicomponent Polymer Systems by Chain-Level Experiments
Presenter: Lance Gill, Chemistry, Oklahoma State University
Authors and Affiliation: Prof. Jeffery L. White Oklahoma State University

Chain-level details about the behavior of pure PI (polyisoprene) and pure PVE (polyvinylethylene), versus their behavior in the miscible blend with one another, are investigated using chain-specific solid-state NMR experiments over a wide temperature range. The PI/PVE blend is a well-known miscible blend, and we compare previous results to those obtained from the experimental strategy we have recently developed (for evaluating miscibility and configurational entropy in saturated polyolefin blends, e.g. Macromolecules 2008, 41, 2832 and 2007, 40, 5433), which employs variable-temperature solid-state magic-angle spinning CODEX NMR experiments to provide chain-specific information for either component in the blend. Even though the PI/PVE blend is miscible, we experimentally verify that the effective glass transitions for each chain type are inequivalent in the blend, and slow segmental dynamics for each polymer in the blend are characterized by unique central correlation times and correlation time distributions. Quantitative analysis of the raw data from the variable-temperature solid-state CODEX NMR methodology indicates that good agreement exists between effective Tg’s, central correlation time constants, correlation time distributions, and friction coefficients extracted from this approach versus those obtained by other methods. That such quantitative information may be obtained for either polymer component in an amorphous mixture, without isotopic labeling, electric dipole moment constraints, or introduction of probe molecules, is a unique advantage of this experimental strategy and illustrates applicability to a wide range of mixed macromolecular systems beyond miscible blends, including polymer nanocomposites, organic/inorganic hybrids, biological macromolecules, and block copolymers.

P63: NMR structural Studies of the C terminal domain of Alpha4, a PP2A regulator
Presenter: Haijuan Du, Biochemistry and Molecular Biology, Oklahoma State University
Authors and Affiliation: Haijuan Du and Michael Massiah, Department of Biochemistry and Molecular Biology, Oklahoma State University, Stillwater OK 74078

Protein phosphatase 2A (PP2A) play a variety of physiological functions that depend on its diverse regulatory subunits. Alpha4 is a subunit that regulates PP2A activity, location, and concentration via ubiquitination. Alpha4 is hypothesized to act as a platform between PP2Ac and the E3 ubiquitin ligase MID1. The N terminal of alpha4 was identified as required for PP2AC binding while the C terminal was shown to interact with the B-box1 domain of MID1. The crystal structure study on the N terminal domain of Tap42, the yeast homolog of alpha4, reveals an all alpha-helical protein and a positively charged region critical for interactions with PP2Ac. However, the structure of C-terminal domain of Alpha4 and how it interacts with the B-box1 domain of MID1 are still unclear. A fragment of Alpha4 consisting of residue Glu236-Leu280 was shown to be sufficient for B-box1 interaction. Here we provide the solution structure of this peptide (alpha45). Our results showed that the free peptide has no obvious structure in aqueous solution. However, it can interact with the Bbox1 domain, suggesting an induced conformation change upon binding. Furthermore Alpha45 forms stable helical structure in the solution with 1% SDS. Based on the interaction surface of B-box1 and the peptide structure in 1% SDS, we hypothesized that binding of B-box1 would induce a helical structure of the C-terminal region of alpha4 that stabilizes the interaction of MID1-alpha4-PP2A. Our results could shed light on the mechanism of the interaction between Alpha4 and MID1.
P64: Solid-State NMR Investigation of Lipid Storage Droplet Protein-1
Presenter: Liying Wang, Physics, Oklahoma State University
Authors and Affiliation: Liying Wang, Estela L. Arrese, Penghui Lin, Lian Duan, Jose L. Soulages, Donghua H. Zhou* Department of Physics, Department of Biochemistry and Molecular Biology, Oklahoma State University, Stillwater, OK 74078, USA

The mechanism by which animals store and utilize neutral lipids triglycerides is complex and not fully understood. Lipid storage droplet protein 1 (Lsd1) is known to regulate the lipolysis of triglycerides. Recently we have shown that Lsd1 can be purified and reconstituted with lipid to study its structure and function in vitro. So far, the three-dimensional (3D) structure of Lsd1 has yet to be determined. Solid-state NMR (SSNMR) is promising to provide the 3D structure and dynamics for such insoluble and disordered protein systems. Here we have initiated NMR study of the structure of Lsd1/DMPG. Analysis of chemical shift dispersion among amino acid types indicate around 50% of α-helix, 10% β-sheet and 40% turn and random coil, in rough agreement with previous circular dichroism analysis. Our preliminary results show that Lsd1/DMPG give good resolution (~0.5 ppm linewidth) and adequate sensitivity, and that SSNMR is the promising tool to elucidate the detailed 3D structure for Lsd1/DMPG and to understand the mechanism of lipid-protein interactions.

8:30 AM - 5:00 PM Ballrooms H and I
Structural Biology Nexus - Posters

P65: In situ Generation of Ferrous Myoglobin Nitrite Using Synchrotron Induced X-Ray PhotoReduction
Presenter: George Richter-Addo, Chemistry and Biochemistry, University of Oklahoma
Authors and Affiliation: Yi Jun University of Oklahoma

It has now been established that humans convert the ubiquitous nitrite anion to the vasodilator nitric oxide (NO). The exact mechanisms of the nitrite-to-NO conversion are not exactly clear, however. We, and others, have shown that the ferrous derivative of the muscle protein myoglobin (Mb) reduces nitrite to NO under anaerobic conditions. We recently prepared, crystallized, and solved the crystal structures of several Mb-nitrite complexes in their ferrous states. Despite various attempts to crystallize the physiologically relevant ferrous Mb-nitrite derivatives, we have not been able to obtain the crystal structure of any ferrous Mb-nitrite complex.

Synchrotron X-rays are much more intense than "home source" X-rays. We have utilized correlated crystallography-spectroscopy techniques at the National Synchrotron Light Source at the Brookhaven National Laboratory in NY to investigate the binding mode of nitrite to the ferrous center of Mb. Specifically, exposure of single crystals of ferric Mb-nitrite to high-intensity X-rays resulted in the generation of the ferrous derivative in very good yields. The crystal structure of this ferrous derivative shows retention of the O-bound nitrite ligand in both the ferric and ferrous forms. This O-binding mode of nitrite is markedly different from all other known hemeprotein-nitrite complexes which show N-binding of nitrite to the metal centers.

P66: Nitrosoalkane Adducts of Human Hemoglobin
Presenter: Guan Ye, Chemistry and Biochemistry, University of Oklahoma
Authors and Affiliation: Jun Yi, George B. Richter-Addo University of Oklahoma

Nitrosoalkanes (R-N=O) are generated in vivo from the oxidative metabolism of amines, or by the reductive metabolism of nitroalkanes. These RNO compounds bind tightly to the Fe centers of various heme proteins and essentially inhibit their normal function by blocking access of other drug metabolites to the Fe sites. Several heme proteins such as hemoglobin (Hb), myoglobin, cytochrome P450, nitric oxide synthase, prostaglandin H synthase, all bind RNO compounds to generate fairly stable heme-RNO derivatives.

We have prepared and characterized by spectroscopy and macromolecular crystallography, new nitrosoalkane adducts of adult human Hb. We show that the RNO ligands bind to the ferrous centers of Hb through the central N-atom. These RNO ligands are not easily displaced from the metal centers. The structures, spectral properties, and structural consequences of RNO binding to the Hb protein will be presented and discussed.

P67: Probing the strand orientation and registry alignment in the propagation of amyloid fibrils
Presenter: Jason Wallace, Chemistry and Biochemistry, The University of Oklahoma
Authors and Affiliation: Wallace, Jason; University of Oklahoma, Chemistry and Biochemistry Shen, Jana; University of Oklahoma, Chemistry and Biochemistry

Detailed knowledge of the structure and growth mechanism of amyloid fibrils is important for understanding the disease process. Recently, solid-state NMR and other spectroscopic data have revealed the equilibrium organization of tertiary structure of fibrils formed by various segments of β-amyloid peptides. A three-step “dock and lock” mechanism for fibril growth has been proposed based on kinetics data. Here we use replica-exchange molecular dynamics simulations to probe the mechanism of tertiary structure propagation in
fibris of Aβ16–22 modeled as an oligomer consisting of two β-sheets each having four strands. The data shows that following association with the oligomer but before being fully locked onto the existing β-sheet, the added monomer predominantly samples states with the anti-parallel strand orientation but both in- and one-residue shifted registry alignments. The in-register state, which is the experimentally observed equilibrium alignment, is marginally more stable than the registry-shifted one. These results suggest that, following the fast docking step, the added monomer dynamically slide in the backbone registry, and stabilization of the preferential registry alignment must occur in the second locking step as the monomer becomes fully integrated with the fibril. We also delineate the electrostatic and hydrophobic effects in directing the registry alignment during monomer addition. Surprisingly, the in-register alignment provides both increased cross-strand electrostatic attraction and hydrophobic surface burial. Finally, our data supports the notion that side-chain hydrophobic burial is a major driving force for β-sheet assembly.

8:30 AM - 5:00 PM Ballrooms H and I
Organic Chemistry - Poster

P68: (±)-1-Alkyl-2-aryl-6-nitro-4-oxo-1,2,3,4-tetrahydroquinoline-3-carboxylate Esters by a Tandem Imine Addition-SNAr Reaction
Presenter: James Schammerhorn, Department of Chemistry, Oklahoma State University
Authors and Affiliation: James E. Schammerhorn and Richard A. Bunce Department of Chemistry, Oklahoma State University

A new tandem imine addition-SNAr reaction has been developed for the synthesis of 1,2,3,4-tetrahydroquinoline-3-carboxylate esters. Several of these esters have been prepared by reacting a series of N-alkylbenzalaldimines with alkyl 3-(2-fluoro-5-nitrophenyl)-3-oxopropanoate. Variation in the final product is possible by changing the structure of the imine or the electron-withdrawing group on the aromatic acceptor. The imines are generated by reaction of a primary amine with 1.2 eq of a substituted benzaldehyde in dimethylformamide. Addition of the β-ketoester then initiates a spontaneous tandem reaction to produce the substituted 1,2,3,4-tetrahydroquinoline-3-carboxylate esters in 73-89% yields. The reaction occurs without the need for added base or heat. To date imines derived from benzaldehyde have given the best results. Future work will include determining conditions that will permit the use of other imines to broaden the scope of the process.

P69: Consistency Among Influences upon Alkene Selenenylation in Chiral Induction, Stereochemistry, Relative Reactivities, and Their Comparisons with Sulfur Analogs
Presenter: Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma
Authors and Affiliation: Donna J. Nelson,* Christopher N. Brammer, and Shanthi Gnananami Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma djnelson@ou.edu

A broad perspective of influences upon alkene selenenylation has been developed by simultaneously considering data for chiral induction, stereochemistry, relative reactivities, and comparison with alkene sulfenylation. Alkyl group branching α to the double bond has the greatest effect of upon chiral induction, stereochemistry, and alkene reactivity. This is in sharp contrast with other additions to alkenes, which depend more upon the degree of substitution on C=C or upon substituent electronic effects. Electronic and steric effects upon chiral induction, stereochemistry, regiochemistry, and relative reactivities in addition of PhSeOTf to alkenes are contrasted and compared against those of PhSCI.

P70: Development of Chiral Zinc Complexes for Esterolytic Kinetic Resolutions: Exploration of Dynamic Combinatorial Catalysis
Presenter: Ramu Kannappan, Chemistry and Biochemistry, University of Oklahoma
Authors and Affiliation: Ramu Kannappan, Masaomi Matsumoto, John Hallren, Kenneth M. Nicholas (Ramu.Kannappan-1@ou.edu and knicholas@ou.edu) Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK, 73019, USA

The use of catalytic asymmetric reactions for the synthesis of enantiomerically enriched chiral compounds is of emergent importance in organic chemistry and in the pharmaceutical industry at large. The primary objective of our work is to determine the viability of catalyst evolution by dynamic templating of metal-ligand complexes with pro-transition state analogs. Herein, we report our preliminary results on the synthesis of chiral 1,2-diaminocyclohexane derivative of imine ligands and their complexes with Zn2+ salts. Interestingly, one of them reveals not only remarkably enhanced catalytic reactivity, but also high enantioselectivity for asymmetric methanolysis of pyridyl esters.
The ethyl 4-oxo-1,4-dihydroquinoline-3-carboxylate scaffold found in several important drug compounds, has been prepared in two steps from ethyl 3-(2-fluorophenyl)-3-oxopropanoate. Treatment of the starting β-ketoester with N,N-dimethylformamide dimethyl acetal gave a nearly quantitative yield of the 2-dimethylaminomethylene-substituted derivative. Reaction of this enammine with a series of primary amines in N,N-dimethylformamide at 140 °C for 2 days then afforded the 4-oxo-1,4-dihydroquinoline-3-carboxylate esters as light tan solids. The yields ranged from 25-70% for the final cyclization, which likely involves a tandem addition-elimination-SNAr reaction. The synthesis of the starting material as well as procedural details and a mechanistic rationale will be presented.

P72: Novel Imageable 3,5-Bis(2-Fluorobenzylidene)-4-Piperidone For PET Imaging
Presenter: Pallavi Lagisetty, Pharmaceutical Sciences, University of Oklahoma Health Sciences Center
Authors and Affiliation: Pallavi Lagisetty,a Kaustuv Sahoo,a Shrikant Ananthb and Vibhudutta Awasthia a Small Animal imaging Facility, College of Pharmacy, OUHSC, Oklahoma City, OK-73117 b Section of Digestive Diseases and Nutrition, Department of Medicine, OUHSC, OKC, OK-73126

The efficacy and safety of curcumin makes it an attractive anticancer therapeutic molecule, but its potential has not been realized because of its poor bioavailability. We synthesized F-18-labeled 2-[3,5-bis(2-fluorobenzylidene-4-piperidonyl)-N-4-fluoro(18F)benzyl]acetamide (FEF) as an imageable anticancer curcuminoid. The non-radioactive analog of FEF was found to be potently anti-proliferative against H441 cells. Since drug distribution may be heterogeneous even in histologically identical tumors, knowledge of drug accumulation in cancer tissue should help in predicting the effect.

P73: One Pot Synthesis of Aryl- and Alkyl-substituted Dihydroquinazolinone Rings By a Dissolving Metal Reduction Process
Presenter: Baskar Nammalwar, Department of Chemistry, Oklahoma State University
Authors and Affiliation: Baskar Nammalwar and Richard A. Bunce, Department of Chemistry, Oklahoma State University

An efficient synthesis of (+)-2-aryl- and 2-alkyl-substituted 2,3-dihydro-4(1H)-quinazolinones has been developed using a dissolving metal reduction-condensative cyclization strategy. Treatment of 2-nitrobenzamide with iron powder in refluxing acetic acid in the presence of an aldehyde or ketone affords high yields of the final target compounds with minimal purification required. More complex ring systems are available by incorporating additional reactive functionality δ to the carbonyl group. The scope and limitations of the process along with optimized procedural details are presented. The same target molecules were also prepared by reaction of 2-aminobenzamide with carbonyl compounds in acetic acid.

P74: Phenylamine Functionalization of Single-Wall Carbon Nanotubes
Presenter: David Martyn, Chemistry and Physics, Southwestern Oklahoma State University
Authors and Affiliation: Logan D. Howard, Shelby C. Josefy, Natalie C. Simpson, David E. Martyn

Single-wall carbon nanotubes were functionalized with phenylamines using dissolving metal reduction and halophenylimines. A number of different reaction methods and procedures were explored to determine which would be the most efficient and reproducible. Lithium metal was used as the electron donor in all reactions with fluoro-, chloro-, bromo-, or iodoaniline serving as the source of the phenylamine functionality. Analysis of the reaction products revealed significant functionalization and the presence of amine functional groups. The products of these reactions will be incorporated into polyimides and polyamides in future studies.
P75: Synthesis of Ferrocene-Modified Polypyrrole for Application as a Molecular Wire in REDOX Polymer Biosensors  
**Presenter:** David Hickey, Chemistry and Biochemistry, University of Oklahoma  
**Authors and Affiliation:** David Hickey, Matthew Meredith, and Daniel Glatzhofer University of Oklahoma, Department of Chemistry and Biochemistry

Conducting polymers have been widely studied for their extensive applications, one of which is their use as glucose biosensors. Polypyrrole is the most studied of the conducting polymers for this application, and it has been shown to act as a mediator between glucose oxidase (GOx) and an electrode. However, transfer of electrons from GOx to polypyrrole is not very efficient as evidenced by the low current densities obtained with biosensors of this type. One possible way around this obstacle is to covalently attach ferrocene to the polypyrrole where it can act as an additional mediator between GOx and the electrode. However, little research has been done on polypyrrole films containing covalently bonded ferrocene compounds. This study will present a comparison of two synthetic methods for the preparation of N-(ferrocenylmethyl)pyrrole and the copolymerization of this compound with various heteroaromatic monomers.

P76: Synthesis of Resveratrol  
**Presenter:** Dustin Sprouse, Biology and Chemistry, Oral Roberts University  
**Authors and Affiliation:** Dustin Sprouse and Lois Ablin, Oral Roberts University, Tulsa, OK

The purpose of this research experiment was to perform and improve the synthesis of resveratrol. Resveratrol (trans-3,4',5-trihydroxystilbene), a natural polyphenolic, non-flavonoid antioxidant, is a phytoalexin found in many plants including grapes, nuts and berries. The Heck reaction was carried out and tested. Several improvements were made to the original decarbonylative Heck reaction.

P77: Toward Consistent Terminology for Cyclohexane Conformers in Introductory Organic Chemistry  
**Presenter:** Donna Nelson, Chemistry & Biochemistry, The University of Oklahoma  
**Authors and Affiliation:** Donna J. Nelson* and Christopher N. Brammer, Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK 73019 djnelson@ou.edu

Recommended changes in use of cyclohexane conformers and their nomenclature will remedy inconsistencies in cyclohexane conformers and their nomenclature, which exist across currently used organic chemistry textbooks. These inconsistencies prompted this logical analysis and the resulting recommendations, which will bring consistency to both. Recommended conformer names are chair, half-chair, twist-boat, and boat. These names are frequently used, although usually combined with additional or alternate names, which can confuse students consulting multiple textbooks. The half-chair conformation structure with 4 coplanar carbons is recommended instead of the one with 5 coplanar carbons, because calculations predict it is more stable and lies on the lowest energy pathway for cyclohexane conformation interconversion. Currently, the incorrect structure with 5 coplanar carbons is most often presented to students. As defined, the recommended names and structures are consistent, descriptive, pedagogically useful, and in agreement with research literature.

8:30 AM - 5:00 PM Ballrooms H and I  
**X-Ray - Poster**

P78: Crystallographic Study of a Novel Cinnamyl Alcohol Dehydrogenase  
**Presenter:** Haiyun Pan, Plant Biology Division, The Samuel Roberts Noble Foundation  
**Authors and Affiliation:** Haiyun Pan, Rui Zhou, Richard A. Dixon, and Xiaoqiang Wang. Plant Biology Division, Samuel Roberts Noble Foundation, 2510 Sam Noble Parkway, Ardmore, OK 73401, USA

The cinnamyl alcohol dehydrogenase (CAD) plays an important role in lignin biosynthesis by catalyzing the reduction of cinnamaldehydes into cinnamyl alcohols, the last step of monolignol biosynthesis before oxidative polymerization in the cell wall. A novel isoform, Medicago MtCAD2, has been identified in Medicago truncatula, which has no significant sequence similarity with other well characterized classic CADs. Medicago MtCAD2 was cloned into pET28a vector and expressed in E. coli. Protein was purified by subsequent nickel-affinity and size exclusion column chromatography. Crystallization screening was carried out. Crystals were obtained using the hanging-drop vapor-diffusion method. The X-ray analysis was carried out, the crystals were found to belong to space group P222, and diffraction data were collected to 2.5 Å resolution. Optimization of crystals and structure determination are in progress. Structural study of CAD will help to understand molecular mechanisms of lignin biosynthesis and facilitate the modification of lignin composition and structure toward improving biomass production and bioconversion efficiency and further enhancing biofuel production.
P79: Preliminary Crystallographic Study of Galactosyltransferase GalT1
Presenter: Qing Chang, Plant Biology Division, The Samuel Roberts Noble Foundation
Authors and Affiliation: Qing Chang, Christopher M. West*, Xiaoqiang Wang. Plant Biology Division, Samuel Roberts Noble Foundation, 2510 Sam Noble Parkway, Ardmore, OK 73401. *) Dept. of Biochemistry & Molecular Biology and Oklahoma Center for Medical Glycobiology, University of Oklahoma Health Sciences Center, Oklahoma City, OK 73104

aGalT1 is a novel UDP-Gal:Fuc alpha-galactosyltransferase encoded by the *agtA* gene from *Dictyostelium* that has been implicated in the regulation of O$_2$-dependent development. It specifically catalyzes the sequential transfer of two galactose residues from UDP-Gal to a hydroxyproline-linked trisaccharide on Skp1, a nucleocytoplasmic protein involved in multiple pathways of cellular regulation. aGalT1 is a novel two-domain protein with an N-terminal catalytic GT77 domain and a C-terminal domain with seven WD-40 repeats. aGalT1 was cloned into pET15TEV vector, expressed in *E. coli* and purified on Ni$^2+$-NTA agarose and gel-filtration columns. Crystallization screening was carried out and crystals were obtained. Preliminary crystallography was carried out and the crystals diffracted weakly to about 7-8Å low resolution. Optimization of crystals is in progress. Structural study of aGalT1 will help to reveal the molecular basis of selective and conditional galactosylation of Skp1, and decipher the enzymatic mechanisms.

P80: Structure function studies of vaccinia virus host-range protein K1 reveal a novel functional surface for ankyrin-repeat proteins
Presenter: Yongchao Li, Biochemistry and Molecular Biology, Oklahoma State University
Authors and Affiliation: Yongchao Li1+, Xiangzhi Meng2+, Yan Xiang2 * and Junpeng Deng1 *
Department of Biochemistry and Molecular Biology, Oklahoma State University, Stillwater, OK1; Department of Microbiology and Immunology, University of Texas Health Science Center at San Antonio, San Antonio, TX2;

Poxvirus host tropism at the cellular level is regulated by virus-encoded host-range proteins acting downstream of virus entry. The functioning mechanisms of most host-range proteins are unclear, but many contain multiple ankyrin (ANK) repeats, a motif that is known for ligand interaction through a concave surface. Here, we report the crystal structure of one of the ANK-repeat-containing host-range proteins, the vaccinia virus K1 protein. The structure, at a resolution of 2.3Å, showed that K1 consists entirely of ANK-repeats, including 7 complete ones and two incomplete ones; one each at the N and C-terminus. Interestingly, Phe82 and Ser83, which were previously shown to be critical for K1’s function, are solvent exposed and locate on a convex surface, opposite to the consensus ANK interaction surface. The importance of this convex surface was further supported by our additional mutagenesis studies. We found that K1’s host-range function was negatively affected by substitution of either Asn51 or Cys47 and completely abolished by substitution of both residues. Cys47 and Asn51 are also exposed on the convex surface, spatially adjacent to Phe82 and Ser83. Altogether, our data showed that K1 residues on a continuous convex ANK-repeat surface are critical for the host-range function, suggesting that K1 functions through ligand interaction and does so with a novel ANK interaction surface.
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