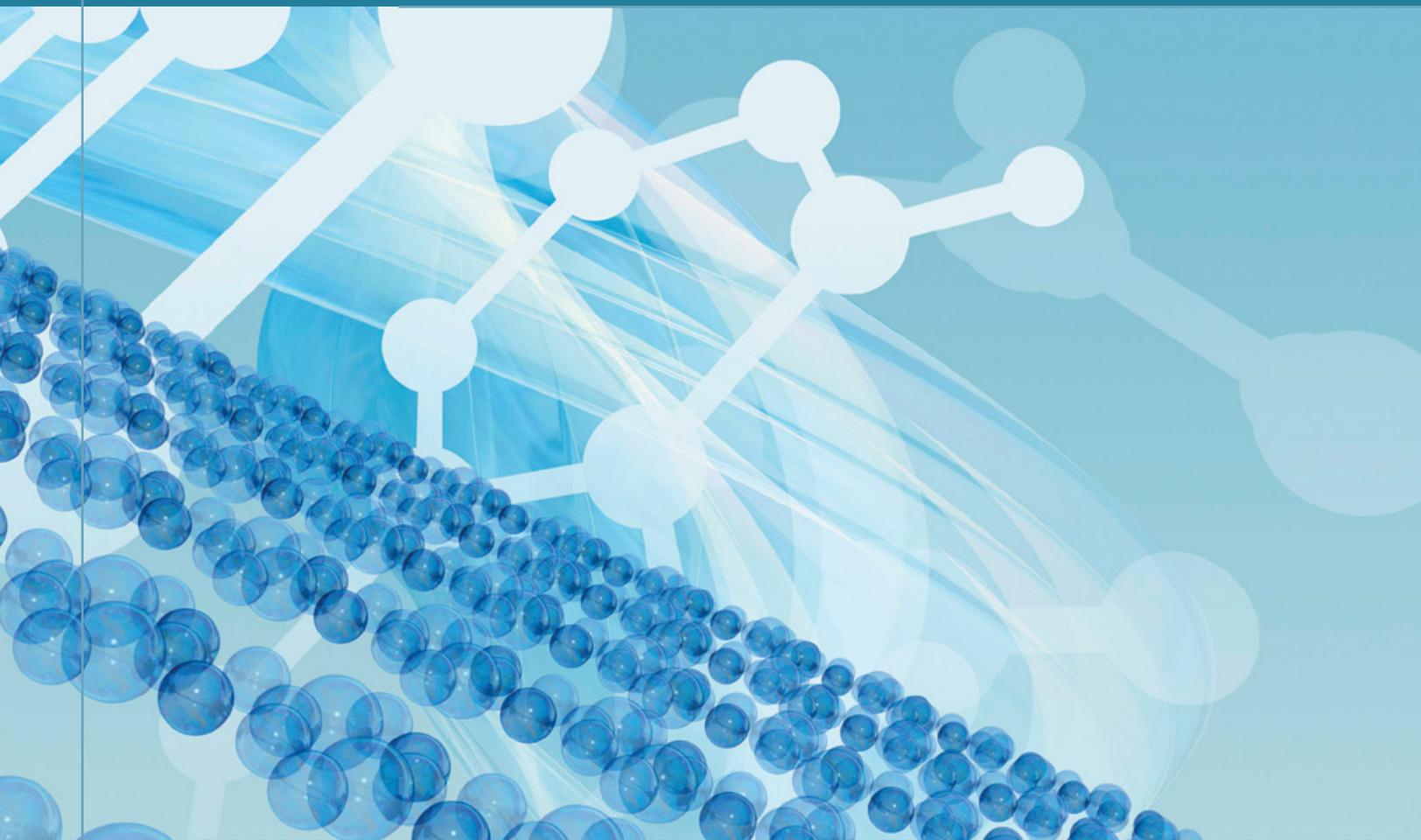


12th Annual Green Chemistry & Engineering Conference



**> *Using Green Chemistry & Engineering
to Advance Sustainable Solutions***

June 23–26, 2008

CAPITAL HILTON ■ WASHINGTON, DC



www.GCandE.org

In appreciation of your attendance at the
**12th Annual Green Chemistry
& Engineering Conference**



We have calculated and off-set the carbon emissions
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with Global ReLeaf resulting in

The planting of 1500 trees.



12th Annual Green Chemistry & Engineering Conference



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Welcome from the Organizing Committee

ON BEHALF OF THE ORGANIZING COMMITTEE, you are cordially invited to join us for the 12th Annual Green Chemistry & Engineering Conference in Washington, DC, June 23–26, 2008.

Using Green Chemistry & Engineering to Advance Sustainable Solutions

The Earth's systems, upon which we all depend, are facing complex and imminent threats. The challenges of global sustainable development, responsible use of resources, and the well-being of the Earth and its inhabitants are intertwined. Green chemistry and engineering are absolutely essential to the development of solutions.

Presenters and attendees at this year's conference will identify and discuss how technical advances in green chemistry and engineering contribute to solutions to some of humanity's most pressing challenges:

- reduce emissions of greenhouse gases and the use of nonrenewable fuel sources
- ensure a safe and adequate food supply
- ensure clean and abundant drinking water
- eradicate disease
- provide new materials to reduce consumption of depletable resources
- improve environmental decision making
- measure progress toward sustainability

Green chemistry and green engineering have enabled tremendous advances in the solution to these significant challenges.

KEYNOTE AND FEATURED SPEAKERS



Dr. Skip Volante
Vice President, Process Research,
Merck & Co. Inc.



Dr. Theodora Colborn
President,
The Endocrine Disruption Exchange (TEDX)



Dr. Steven Chu
Director,
Lawrence Berkeley National Laboratory



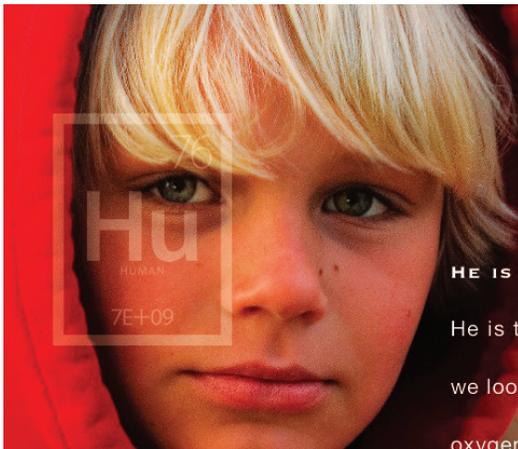
Dr. Bill Banholzer
Chief Technology Officer,
The Dow Chemical Company



Jonathan Lash
President,
World Resources Institute



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oxygen and carbon we see solutions for problems facing

the planet. From clean water to affordable housing to

climate change. The work of chemistry is the work of

humanity. That's how we see things at The Dow Chemical

Company. Through the eyes of the Human Element.

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ACS NATIONAL MEETING & EXHIBITION "Chemistry for Health: Catalyzing Translational Research"



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AIChE—Institute for Sustainability

2008 Organizing Committee

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Tamara J. Nameroff, Chair
ACS Green Chemistry Institute

Martin Abraham
Youngstown State University

Sharon Austin
U.S. Environmental Protection Agency

Diana Bauer
U.S. Environmental Protection Agency

Ellyn Beary (Lyn)
National Institute for Standards and Technology

Rich Engler
U.S. Environmental Protection Agency

Julie Haack
University of Oregon

Carole A. LeBlanc
Department of Defense

Julie Manley
ACS Green Chemistry Institute Pharmaceutical Roundtable

Carl Maxwell
American Chemical Society

Cynthia Nolt-Helms
U.S. Environmental Protection Agency

Darlene Schuster
AIChE Institute for Sustainability

Megan Turner
BASF

Anne Wallin
The Dow Chemical Company

CONFERENCE ADMINISTRATORS

Jane Day
Jesse Gallun
Beverly Johnson
Joyce Kilgore
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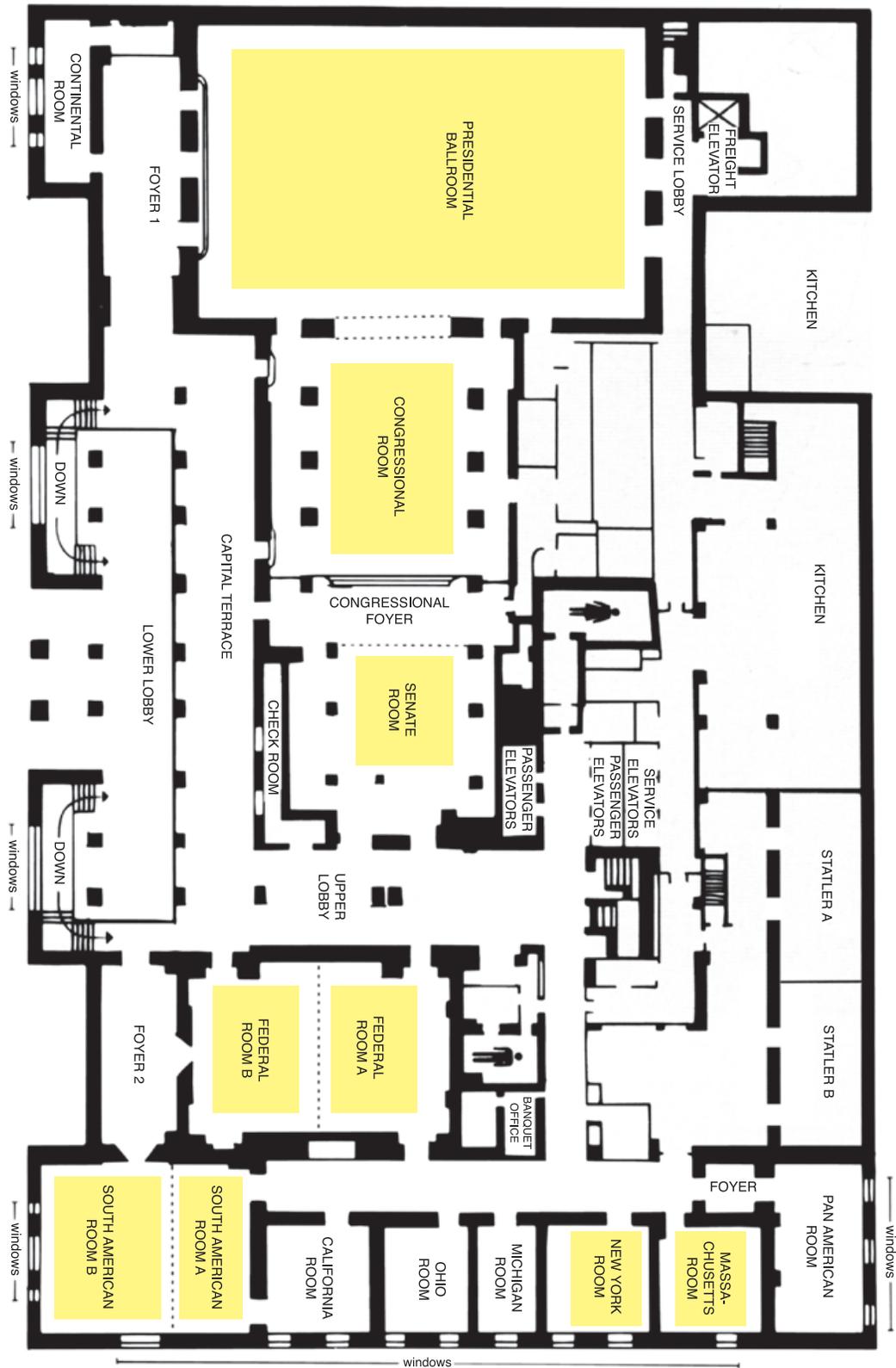
Schedule at a Glance

	MORNING	
MONDAY, June 25	<p>Student Workshop <i>(The student workshop is free to all students registered for the conference. Lunch provided.)</i></p> <p>This full-day workshop is designed for undergraduate, graduate, and post-doctoral students interested in green chemistry and engineering. Expert green chemistry and engineering researchers in industry and academia will make presentations and lead small-group discussions.</p> <p>ACS GCI Pharmaceutical Roundtable Meeting <i>(by invitation only)</i></p>	
TUESDAY, June 26	 <p>KEYNOTE: Skip Volante, PhD, Vice-President, Process Research, Merck & Co.</p>	<ul style="list-style-type: none"> ■ Analytical Methods & Technologies ■ Bio-Based Materials & Processes ■ Environmental Decision Making & Metrics ■ Greenhouse Gas Emission Reduction and Trading in North America: How Can the Chemical Sector Engage? <p>EXHIBITS</p>
WEDNESDAY, June 27	<p>OPENING SESSION: Perspectives from Winners of the 2008 Presidential Green Chemistry Challenge Awards</p>  <p>KEYNOTE: Theodora E. Colborn, PhD, President, The Endocrine Disruption Exchange (TEDX)</p>	<ul style="list-style-type: none"> ■ Presidential Green Chemistry Challenge Award Winners ■ Bio-Based Materials & Processes ■ Education & Outreach ■ Process Design <p>EXHIBITS</p>
THURSDAY, June 28	 <p>KEYNOTE: Steven Chu, PhD, Director, Lawrence Berkeley National Laboratory</p>	<ul style="list-style-type: none"> ■ Catalysis ■ Education & Outreach ■ New Materials

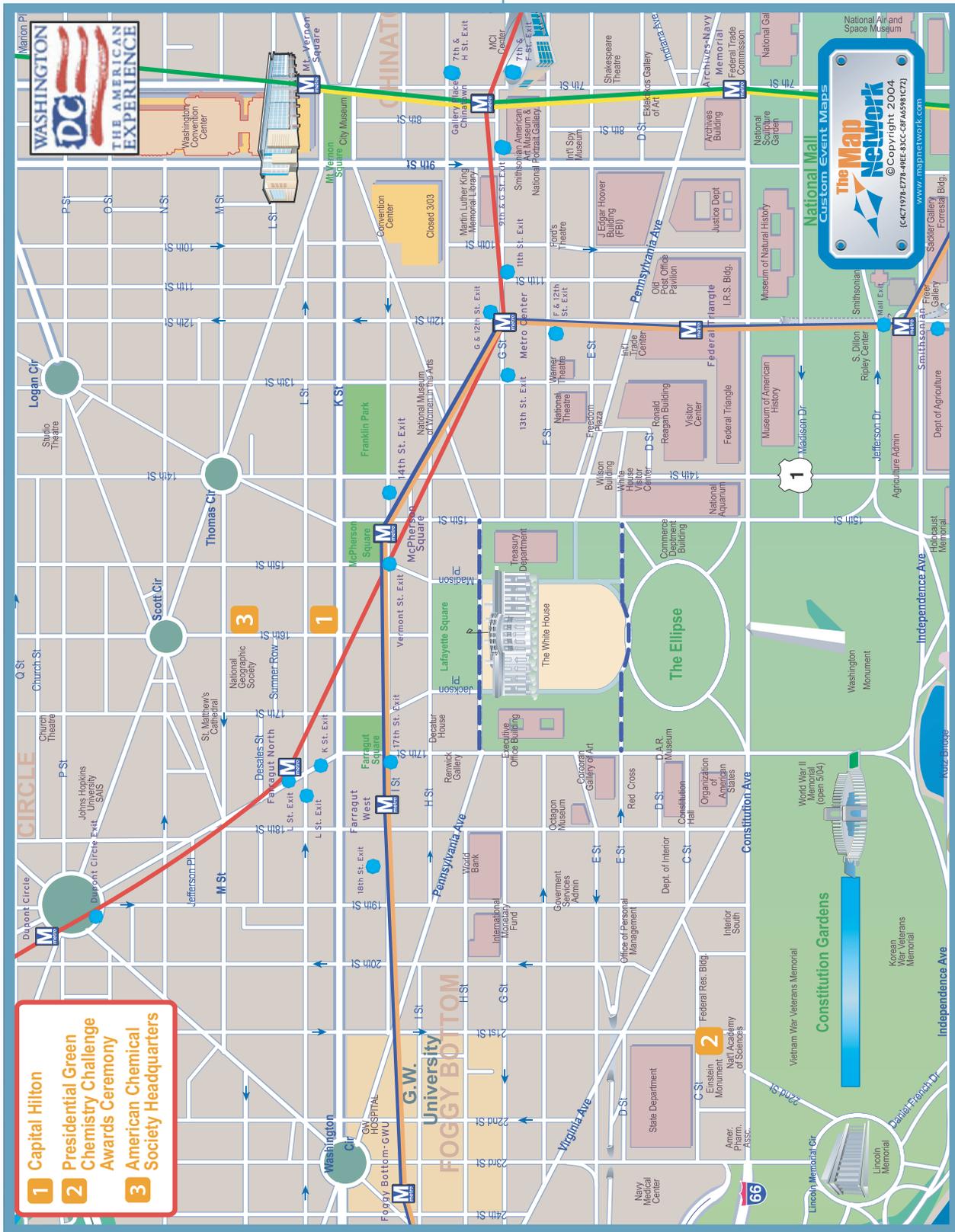


AFTERNOON	EVENING
<p>Student Workshop <i>(Continued)</i></p> <p>ACS GCI Pharmaceutical Roundtable Meeting <i>(by invitation only)</i></p>	
<ul style="list-style-type: none"> ■ Bio-Based Materials & Processes ■ Environmental Decision Making & Metrics ■ Solvents & Solvent Systems ■ Synthesis <p>EXHIBITS</p>	<p>Presidential Green Chemistry Challenge Awards Ceremony <i>(free but pre-registration required)</i></p> <p>Conference participants are cordially invited to attend this ceremony at 5:30 PM at the National Academies, 2100 C Street, NW, Washington, DC</p> <p>Business attire required.</p>
 <p>LUNCHEON</p> <p>Luncheon Speaker: Bill Banholzer, PhD, Chief Technology Officer, The Dow Chemical Company</p> <ul style="list-style-type: none"> ■ Catalysis ■ Environmental Decision Making & Metrics ■ Process Design ■ Synthesis ■ Natural Capitalism ■ KeLa Energy Clean Coal Technology <p>POSTER RECEPTION</p> <p>EXHIBITS</p>	 <p>BANQUET</p> <p>Banquet Speaker: Jonathan Lash, President, World Resources Institute</p>
<ul style="list-style-type: none"> ■ Catalysis ■ Education & Outreach ■ New Materials <p>CLOSING SESSION</p>	

Capital Hilton Floorplan — Second Floor



Washington Area Map



Track Descriptions & Leaders

ANALYTICAL METHODS AND TECHNOLOGIES:

Sessions will examine advances in assessing analytical methodologies within the context of green chemistry, novel in-situ measurement techniques, energy efficient separation techniques, and process analytical chemistry to provide real-time monitoring. Presentations on the latest advances in techniques and technologies are welcomed.

TRACK LEADER: Douglas Raynie, South Dakota State University

BIO-BASED MATERIALS AND PROCESSES:

Sessions will cover how bio-based and renewable materials such as sugars and starches are substituting for petrochemical building blocks to revolutionize chemical manufacturing. Contributions are encouraged in the conversion of biomass (agricultural waste products, carbohydrates, proteins, fats, terpenoids) into industrially viable products, and the use of carbon dioxide as a new feedstock, and discussion of scale-up into industrial processes.

TRACK LEADER: Richard Wool, University of Delaware

CATALYSIS:

New methods to reduce the energy intensity of chemical processes with catalysts that are highly selective and provide rapid reaction times without the use of substances as hazardous to humans and the environment. Attendees will learn about advances in the development of multifunctional catalysts, novel catalysts with preferential solubility in green solvents, single-site catalysis, catalyst separation and recycling, use of enzymes in novel chemical transformations, mechanisms of enzymatic reactions in the design of biomimetic analogues, single-site heterogeneous catalysts, substrate-selective conversion of complex materials, design and synthesis of chiral catalysts and novel catalytic materials. Engineering and commercialization issues also will be addressed.

TRACK LEADER: John Regalbuto, National Science Foundation

EDUCATION AND OUTREACH:

Sessions will highlight recent innovations in green chemistry education and outreach activities, including new pathways for academic/industrial collaboration, educational materials, information resources, and assessment. Contributors will provide ideas for incorporating green chemistry throughout diverse teaching and learning environments.

TRACK LEADER: Julie Haack, University of Oregon

ENVIRONMENTAL DECISION MAKING AND METRICS:

Sessions will cover issues related to the assessment of sustainable processes. Topics to be covered include greening the supply chain, life-cycle assessment of energy systems and materials, metrics and benchmarking, and government policies that could advance or hinder adoption of green chemistry and engineering technologies. Contributions also are welcomed in methods to assess toxicity and sustainability in the absence of complete information.

TRACK LEADER: Richard Helling, The Dow Chemical Company and Olivier Joliet, University of Michigan

NEW MATERIALS:

Sessions will cover polymers, green nanotechnology, and advances in fundamental understanding of achieving the same or better product performance with less material (e.g., thinner polymers, higher biological activity, better stability, etc.).

TRACK LEADER: Megan Turner, BASF

PROCESS DESIGN:

Sessions will cover new developments in green process design, green reaction metrics, green manufacturing strategies, and energy efficient technologies. Contributions also are welcomed in areas such as reaction modeling, scale-up rules, and reactor engineering.

TRACK LEADERS: Julie Manley, ACS Green Chemistry Institute Pharmaceutical Roundtable and Richard Engler, U.S. Environmental Protection Agency

SOLVENTS AND SOLVENT SYSTEMS:

Sessions will cover biobased solvents, benign solvents, alternative solvents such as ionic liquids and fluorinated media, supercritical fluids, "smart solvents" that sense certain conditions, such as heat, and are designed to respond accordingly, "obedient solvents" that change basic physical and chemical properties as a response to an imparted stimulus, new applications for water-based solvent systems, and "greener" organic solvents, which can be derived from renewable feedstocks or can be designed at the molecular level to have reduced environmental impact.

TRACK LEADERS: Julie Manley, ACS Green Chemistry Institute Pharmaceutical Roundtable and Joan Brennecke, University of Notre Dame

SYNTHESIS:

Sessions will cover biological transformations, chemical transformations that minimize energy input, reactivity and toxicity in the design of synthetic methods, synthesis in aqueous systems, strategies to impart new properties and performance in molecules and materials, direct derivatization and elimination of substitution reactions, and design for degradation and recyclability.

TRACK LEADERS: Julie Manley, ACS Green Chemistry Institute Pharmaceutical Roundtable and Richard Engler, U.S. Environmental Protection Agency





Monday, June 23, 2008
Green Chemistry & Engineering Student Workshop
 (pre-registration required)

7:30 AM – 8:30 AM		Continental Breakfast	
8:30 AM – 5:00 PM		American Chemical Society, Marvel A/B/C	
STUDENT WORKSHOP SCHEDULE ORGANIZERS: L. Gron, Ph.D. and J. Kilgore			
8:30 AM	Welcome and Introductions <i>Liz Gron, PhD, Hendrix College</i> <i>Joyce Kilgore, ACS Green Chemistry Institute</i>	1:00 PM	Green Nanomaterials <i>Jim Hutchison, PhD, University of Oregon</i>
8:40 AM	Opening Remarks <i>Tamara Nameroff, PhD, GC&E Conference Chair</i>	1:40 PM	Group Discussion
8:50 AM	Green Sustainability <i>John Warner, PhD</i> <i>Warner-Babcock Institute for Green Chemistry</i>	2:00 PM	Green Chemistry in the Pharmaceutical Industry: Accomplishment and Opportunities <i>Berkeley "Buzz" Cue, PhD, Private Consultant</i>
9:30 AM	Green Innovation <i>Eric Beckman, PhD, University of Pittsburgh</i>	2:40 PM	Tea & Coffee Break
10:10 AM	Group Discussion	3:00 PM	Making It Happen: Resources and Strategies for Getting Green Chemistry Into the Classroom <i>Julie Haack, PhD, University of Oregon</i>
10:35 AM	Tea & Coffee Break	3:40 PM	Group Discussion
10:50 AM	Industrial Applications of Green Chemistry <i>Amy Cannon, PhD, Beyond Benign</i>	4:00 PM	The Big Picture: Why Green Chemistry and Green Engineering are Important <i>Paul Anastas, PhD, Yale University</i>
11:30 AM	Group Discussion	4:30 PM	Closing Remarks <i>Bob Peoples, PhD,</i> <i>Director, ACS Green Chemistry Institute®</i>
12:00 PM	Lunch, Marvel E/F		

Technical Program

Tuesday, June 24, 2008

Tuesday Morning

7:45 AM – 8:45 AM

Continental Breakfast

UPPER LOBBY (CAPITAL HILTON)

7:45 AM – 4:30 PM

Exhibition

CAPITAL TERRACE (CAPITAL HILTON)

7:00 AM – 8:00 PM

Registration

FOYER 1 (CAPITAL HILTON)

8:45 AM – 9:00 AM

Welcome Remarks

PRESIDENTIAL BALLROOM (CAPITAL HILTON)



9:00 AM – 10:00 AM

KEYNOTE ADDRESS: Skip Volante

Vice President, Process Research, Merck & Co. Inc.

“Green Challenges and Accomplishments in the Pharmaceutical Industry”

PRESIDENTIAL BALLROOM (CAPITAL HILTON)

10:00 AM – 10:30 AM

Tea and Coffee Break

UPPER LOBBY (CAPITAL HILTON)

ANALYTICAL METHODS AND TECHNOLOGIES

10:30 AM – 12:10 PM

Analytical Methods and Technologies

NEW YORK (CAPITAL HILTON)

SESSION CHAIR: Douglas Raynie, South Dakota State University

- 10:30** 1 A Green Chemistry Assessment for Analytical and Chemical Processes. **Julee Driver**¹, Douglas Raynie¹ and Paul Jackson², (1)South Dakota State University, (2) St. Olaf College
- 10:50** 2 Instructional Resources for the Teaching of Green Analytical Chemistry. **Douglas Raynie**, South Dakota State University
- 11:10** 3 Micro-Scale HPLC Generates < 1% of the Solvent Waste of Conventional Analytical LC. **Justin E. Kittell**, Phil Paul, Don Arnold, Dave Neyer, Phil DeLand and Jason Rehm, Eksigent Technologies
- 11:30** 4 Direct Analysis in Real Time (DART)/ High Resolution Mass Spectrometry: Green Chemistry Applications. **Ted H. E. Mendum** and John C. Warner, Warner Babcock Institute for Green Chemistry

- 11:50** 5 Green Product Design of Temperature Sensors. **Maria Nydia Ruiz Felix**, Robert P. Hesketh, Robert Newland and Darius Kuciauskas, Rowan University

BIO-BASED MATERIALS AND PROCESSES

10:30 AM – 12:10 PM

Bio-Based Materials: Session I

FEDERAL ROOM A (CAPITAL HILTON)

SESSION CHAIR: Richard P. Wool, University of Delaware

- 10:30** 6 Rapid Evaluation and Functional Design of SMB Chromatography for Separation of Vegetable Oil-Derived Hydroxy Methyl Esters. **Shawn D. Feist**, Bruce W. Pynnonen, Timothy C. Frank and Zenon Lysenko, The Dow Chemical Company
- 11:10** 7 Fractionation of Lignocellulosic Biomass Feedstocks. **Lisette Ngo Tenlep** and Doug Raynie, South Dakota State University
- 11:30** 8 System for Bioremediation of Effluents. **John R. Roheim**, NCH Corporation
- 11:50** 9 Liquid Carbon Dioxide-Based Production of Leather. **Doug Raynie** and **Jeremy Kroon**, South Dakota State University

ENVIRONMENTAL DECISION MAKING AND METRICS

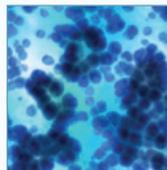
10:30 AM – 12:10 PM

Federal Metrics and Policy

SOUTH AMERICAN AB (CAPITAL HILTON)

SESSION CHAIR: Richard Helling, The Dow Chemical Company

- 10:30** 11 “Green” Comparisons for Functionally Equivalent Products in Federal Supply Catalogs. **George R. Thompson**, Chemical Compliance Systems, Inc. and Raymond Paulson, Fleet Readiness Center Southwest North Island
- 10:50** 12 The Importance of Chemical Ranking Systems: A Department of Defense Study. **Carole A. LeBlanc**, Office of the Deputy Under Secretary of Defense
- 11:10** 13 Characterizing and Addressing Policy Barriers to Green Chemistry in the United States. **Michael P. Wilson** and Megan R. Schwarzman, MD, MPH, University of California, Berkeley
- 11:30** 117 Pulling down the Barriers: Lessons from Local and International Variations in Green Chemistry Policy. **Kira JM Matus**, Harvard University



INVITED PAPERS

10:30 AM – 12:10 PM

Greenhouse Gas Emission Reduction and Trading In North America: How Can the Chemical Sector Engage?

FEDERAL ROOM B (CAPITAL HILTON)

- 10:30** 14 Greenhouse Gas Emission Reduction and Trading In North America: How Can the Chemical Sector Engage? **Kellee James**, Chicago Climate Exchange

12:10 PM – 1:30 PM

Lunch Break (*on your own*)

Tuesday Afternoon

BIO-BASED MATERIALS AND PROCESSES

1:30 PM – 4:30 PM

Bio-Based Materials: Session II

FEDERAL ROOM A (CAPITAL HILTON)

SESSION CHAIR: Victor Atiemo-Obeng, The Dow Chemical Company

- 1:30** 15 Characteristics and Performance of a Wood Preservative Produced from Pyrolysis Oil. **Philip H. Steele**, El-Barbary Hassan, Jerome E. Cooper, Christopher V. Ruhs and Leonard L. Ingram, Mississippi State University
- 1:50** 17 Bio-Based Composites: Design for Commercialization. **Richard P. Wool**, University of Delaware
- 2:10** 18 Natural Oil Polythiols and Their Utility in Polymeric Systems. **Chad W. Brown**, Chevron Phillips Chemical Company, LP
- 2:30** 19 L'OREAL's Commitment to Green and Sustainable Chemistry. **Michel D. Philippe**, L'OREAL
- 2:50** 20 Recent Advances in Green Chemistry Research & Development as Sources for New Eco-Friendly Materials Protection Agents. **Walter Bogaerts¹, Thuy Vu thi¹, Abdul Rauf¹, Quoc Hung Le², Hong Phong Pham², Hong Hanh Pham² and Chi Linh Do²**, (1)University of Leuven, (2) Vietnamese Academy of Science and Technology (VAST)
- 3:30** 21 Fatty Acid-Based Monomer as a Replacement for Styrene in the Production of Triglyceride-Based Polymers. **Alejandrina Campanella¹, John J. La Scala² and Richard P. Wool¹**, (1)University of Delaware, (2)Army Research Labs
- 3:50** 22 Bioplastic Blends and Nanocomposites: New Green Materials. **John R. Dorgan¹, Margaret Sobkowicz¹, Rakhi Patel¹ and Birgit Braun²**, (1)Colorado School of Mines, (2) PolyNew Inc

SOLVENTS AND SOLVENT SYSTEMS

1:30 PM – 3:10 PM

Ionic Liquids

FEDERAL ROOM B (CAPITAL HILTON)

SESSION CHAIR: Megan Turner, BASF Corporation

- 1:30** 23 Ionic Liquids for Absorption Refrigeration. **Joan F. Brennecke** and **Lindsay E. Ficke**, University of Notre Dame
- 1:50** 25 Industrial Use of Ionic Liquids—Challenges and Opportunities. **Peter FH Schwab**, **Matthias Seiler** and **Bernd Weyershausen**, Evonik Degussa
- 2:10** 26 Water-in-Ionic Liquid Microemulsions: A New Medium for Biocatalytic Reactions. **Muhammad Moniruzzaman**, **Noriho Kamiya** and **Masahiro Goto**, Kyushu University
- 2:30** 27 Surface Structure and Green Chemistry in the Organic Solid State. **John C. Warner** and **Donna Guarrera**, Warner Babcock Institute for Green Chemistry

ENVIRONMENTAL DECISION MAKING AND METRICS

1:30 PM – 4:30 PM

Methodologies for Assessment and Sustainability

SOUTH AMERICAN AB (CAPITAL HILTON)

SESSION CHAIR: Richard Helling, The Dow Chemical Company,

- 1:30** 28 Comparative Assessment of Chemicals Impacts on Ecosystems and Human Health Using the USEtox Model. **Olivier Jolliet¹, Michael Hauschild², Mark Huijbregts³, Manuele Margni⁴, Thomas McKone⁵, Matt MacLeod⁶, Dick Van de Meent⁷ and Ralph Rosenbaum⁴**, (1)University of Michigan, (2)Technical University Denmark, (3)Radboud University, (4)Ecole Polytechnique de Montreal, (5) University of California—Berkeley, (6)Swiss Federal Institute of Technology Zuerich, (7)RIVM
- 2:10** 29 A Methodology for Driving Environmental Improvements in the Process Development of Active Pharmaceutical Ingredients. **James A. Baird**, **Stephen Evans**, **Mark Hoyle**, **Magnus Bergqvist** and **Daniel J. Horner**, AstraZeneca
- 2:30** 30 Developing Proactive Design Strategies in Nanoscience to Reduce Uncertainty, Enhance Performance and Minimize Hazard. **Bettye L.S. Maddux¹, Stacey L. Harper², Robert T. Tanguay² and James E. Hutchison³**, (1)Safer Nanomaterials and Nanomanufacturing Initiative, (2) Oregon State University, (3)University of Oregon
- 2:50** 31 BASF's Socio-Eco-Efficiency Analysis: A Method for Evaluating the Economic, Environmental and Social Impacts of Products. **Christopher A. Bradlee**, BASF Corporation
- 3:10** Break
- 3:30** 32 Benchmarking Sustainability. **Darlene Schuster**, AIChE Institute for Sustainability, **Subhas Sikdar**, US EPA and **Calvin B. Cobb**, Institute for Sustainability
- 3:50** 33 Environmental Decision Making & Metrics: Methodologies for Assessment & Sustainability. **Sharon Austin**, Environmental Protection Agency (U.S. EPA)

Technical Program, *Continued*

SYNTHESIS

1:30 PM – 4:30 PM

Synthetic Methods

NEW YORK (CAPITAL HILTON)

SESSION CHAIR: Miles Fabian, NIGMS/NIH

- 1:30** 35 Metal and Organic Solvent Free Green Oxidation of Alkyl Substituted Aromatics to Ketones and Carboxylic Acids with Aqueous Tert-Butyl Hydroperoxide Under Microwave Irradiation. **Albert W. M. Lee**, Hao He and Bao-Jian Pei, Hong Kong Baptist University
- 1:50** 36 Greener and Rapid Synthesis of Bio-Active Heterocycles. **Vivek Polshettiwar** and Rajender, S. Varma, US EPA
- 2:10** 37 The “Greener” Leuckart Reaction. **Mikhail M. Bobylev** and Lioudmila I. Bobyleva, Minot State University
- 2:30** 38 Fluorous Separation and Recycling Technologies for Green Organic Synthesis. **Wei Zhang**, University of Massachusetts-Boston
- 2:50** 39 Developing “Greener” Synthesis through Mechanochemistry. **James Mack**, Daniel C. Waddell, William C. Shearouse II, Maxwell Shumba and Philip A. Vogel, University of Cincinnati
- 3:10** Break
- 3:30** 40 Stabilized Alkali Metals for Safer, Sustainable Synthesis. **Paul Vogt¹**, Michael Lefenfeld¹ and Partha Nandi², (1)SiGNa Chemistry, Inc., (2)Michigan State University
- 3:50** 41 A Clean, Benign and Aqua Mediated Synthesis of Pharmacologically Active Spiro Heterocycles. **Subhash C. Jain**, Siva Panda, Pankaj Khanna and Sunita Bhagat, University of Delhi

SOLVENTS AND SOLVENT SYSTEMS

3:30 PM – 4:30 PM

Alternative Solvents

FEDERAL ROOM B (CAPITAL HILTON)

SESSION CHAIR: Joan F. Brennecke, University of Notre Dame

- 3:30** 42 Terephthalic Acid Synthesis at Higher Concentrations in High-Temperature Liquid Water. Mitsumasa Osada, Ichinoseki National College of Technology and Phillip E. Savage, University of Michigan
- 3:50** 43 Piperylene Sulfone: A Fully Recyclable Smart Solvent to Couple Reactions and Separations. **Veronica Llopis-Mestre**, Daniele Vinci, Megan Donaldson, Pamela Pollet, Charles Liotta and Charles Eckert, Georgia Institute of Technology
- 4:10** 44 Novel Biomimetic Catalysts for Green Polymerization in Water. **Kei Saito**, Monash University

Tuesday Evening

5:30 PM – 7:30 PM

Presidential Green Chemistry Challenge Awards Ceremony

NATIONAL ACADEMIES, 2100 C STREET, NW, WASHINGTON DC

Business dress. Pre-registration required.

Wednesday, June 25, 2008

Wednesday Morning

7:00 AM – 7:30 AM

Continental Breakfast

UPPER LOBBY (CAPITAL HILTON)

7:00 AM – 5:30 PM

Exhibition

CAPITAL TERRACE (CAPITAL HILTON)

7:00 AM – 5:30 PM

Registration

FOYER 1 (CAPITAL HILTON)

7:30 AM – 8:30 AM

Opening Session: Perspectives from Winners of the 2008 Presidential Green Chemistry Challenge Awards

PRESIDENTIAL BALLROOM (CAPITAL HILTON)

SESSION CHAIR: Paul Anastas, Center for Green Chemistry and Green Engineering at Yale



8:30 AM – 9:30 AM

KEYNOTE ADDRESS: Theo Colborn

President, The Endocrine Disruption Exchange (TEDX)

“The Male Predicament”

PRESIDENTIAL BALLROOM (CAPITAL HILTON)

9:30 AM – 10:00 AM

Tea and Coffee Break

UPPER LOBBY (CAPITAL HILTON)

BIO-BASED MATERIALS AND PROCESSES

10:00 AM – 12:00 PM

Bio-Based Materials: Session III

FEDERAL ROOM A (CAPITAL HILTON)

SESSION CHAIR: John R. Dorgan, Colorado School of Mines

- 10:00** 45 Novel Biocomposites from the Fibers of Poultry Feather and Biopolymer. **Masud Huda¹**, Walter F. Schmidt² and Marc Teffeu¹, (1)Horticultural Research Institute, (2) USDA/ARS/EMBUL

- 10:20** 46 Bio-Based Dielectric Materials for Printed Circuit Boards. **Mingjiang Zhan** and Richard P. Wool, University of Delaware
- 10:40** 47 Hydrogen Storage on Carbonized Chicken Feather Fibers. **Erman Senoz** and Richard P. Wool, University of Delaware
- 11:00** 48 Renewable CARBON Nanospheres for Applications in Polymer Nanocomposites. **Margaret Sobkowicz**, John R. Dorgan, Keith W. Gneslin, Andrew M. Herring and J. Thomas McKinnon, Colorado School of Mines
- 11:20** 49 Cellulosic Nanowhiskers: One-Step Functionalization and Use in Ecologically Benign Nanocomposites. **Birgit Braun**, PolyNew Inc and John R. Dorgan, Colorado School of Mines
- 11:40** 50 DuPont™ Cerenol™—a New Family of Sustainable and Environmentally Friendly Materials. **Hari B. Sunkara**, E. I. du Pont de Nemours and Company

PROCESS DESIGN

10:00 AM – 12:00 PM

Industrial Process Design

NEW YORK (CAPITAL HILTON)

- 10:00** 51 Elimination of Hexavalent Chromium Used in Hydraulic & Pneumatic Tubing. **Robert R. Rick**, Commercial Fluid Power
- 10:20** 52 Improved Control of Organic Sulfur. **Stephen A. Bedell**, The Dow Chemical Company
- 10:40** 53 A Novel Solid Catalyst Process for Biodiesel Production. **Dheeban Kannan** and Jack V. Matson, The Pennsylvania State University
- 11:00** 54 Developments in REACTOR Engineering: MODELING of Gas—Phase Catalytic Channel Reactors. **Alex Omo Ibhado**¹, Polycarpus Falaras² and Dimitris Tsoukleris², (1) University of Hull, (2)Institute of Physical Chemistry
- 11:20** 55 Extension of the Environmentally Benign Catecholate Method to the Synthesis of Barium-Based Perovskites and Environmentally Benign Synthesis of Doped Barium Titanate. **Anne E. Marteel-Parrish**, Danielle Harlan, Jonathan Martin, Samantha DeCarlo and Heather Sheridan, Washington College
- 11:40** 56 Biomass-to-Liquids (BTL): The Green Fuel of the Future? **Jeff McDaniel** and Dave Kilanowski, Velocys, Inc.

10:00 AM – 12:00 PM

Presidential Green Chemistry Challenge Awards

SOUTH AMERICAN AB (CAPITAL HILTON)

SESSION CHAIR: Rich Engler, US Environmental Protection Agency

EDUCATION AND OUTREACH

10:00 AM – 12:00 PM

Education and Outreach: Session I

FEDERAL ROOM B (CAPITAL HILTON)

SESSION CHAIR: Michael C. Cann, University of Scranton

- 10:00** 58 Greening Analytical Chemistry Education: Expanding the Green Revolution. **Liz Gron**, Hendrix College
- 10:20** 59 Development of a Green Inorganic Chemistry Laboratory: Principles, Practices and Procedures. **Indu Tucker Sidhwani**, Gargi College, University of Delhi and R.K. Sharma, University of Delhi
- 10:40** 60 An Undergraduate Research Experience in Green Chemistry: Exploring An Immobilization Strategy for a Heterogeneous Catalyst. **Corey A. Mocka** and **Denyce K. Wicht**, Suffolk University
- 11:00** 61 “Greening up” Organic Reactivity in the Undergraduate Laboratory: Aqueous Horner-Wadsworth-Emmons, Heck and Suzuki Reactions. **Andrew P. Dicks**, University of Toronto
- 11:20** 62 Green Chemistry Networking in India. **R. K. Sharma**, University of Delhi
- 11:40** 63 Infusing Sustainability and Additional Green Chemistry into Chemistry in Context. **Michael C. Cann**, University of Scranton



12:00 PM – 1:00 PM

LUNCHEON AND GUEST SPEAKER: **Bill Banholzer**

Chief Technology Officer, The Dow Chemical Company

What Can Chemists and Chemical Engineers Do about Greenhouse Gases?

SENATE (CAPITAL HILTON)

Wednesday Afternoon

Poster Session (Bio)

SESSION CHAIR: Darlene Schuster, AIChE Institute for Sustainability

1:00 PM – 2:00 PM

CONGRESSIONAL ROOM (CAPITAL HILTON)

BIO-BASED MATERIALS AND PROCESSES

- 64 A Study of Ganoderma Amboinense Lanostanoid Triterpene. **Lou-sing Kan** and Hung-Chieh Lu, Academia Sinica
- 65 Commercial Viable Resolution of (S)-Ibuprofen. **David Chavez** and James Salvador, University of Texas at El Paso
- 66 Soy-Based Polyols for Polyurethane Applications. **Zuleica Lozada** and Galen J. Suppes, University of Missouri-Columbia
- 67 Use of Highly Nanoporous Carbon in Batteries and Supercapacitors. **Sean P. Crockett**, Ali Tekeci, Michael Gordon, Bryan D. Sawyer, Matt Wopata and Galen J. Suppes, University of Missouri-Columbia
- 68 Photocatalytic Degradation of Omethoate Using Ti-Containing Zeolite. **Dishun Zhao** and Jialei Wang, Hebei University of Science and Technology

Technical Program, *Continued*

- 69 Surface Modified Silica Supported Zinc Salicylaldimine Complex for Use as Catalyst in Transesterification: A Green Chemistry Approach. **Anju Srivastava**, R.K. Sharma and Deepti Rawat, University of Delhi
- 70 Chemically Modified Fatty Acid Methyl Ester and Its Use in Vinyl Ester Resins. **Alejandrina Campanella**, Gregory Stirparo, Michael Zeberkiewicz and Richard P. Wool, University of Delaware
- 71 Green Engineering Design for the Recovery of Solvents in API Manufacturing. **Anthony J. Furiato**, **Kyle E. Lynch**, **Timothy M. Moroz**, **Mariano J. Savelski** and **C. Stewart Slater**, Rowan University
- 72 Bodied Soybean Oil Hydroxylation Via Transesterification. **Arnold Lubguban**, **Yuan-Chan Tu**, **Zuleica Lozada**, **Fu-hung Hsieh** and **Galen J. Suppes**, University of Missouri-Columbia
- 73 Mechanical Properties of Water-Blown Flexible Polyurethane Foams Containing Epoxidized Soybean Oil. **Yuan-CHAN TU**, **Hongyu Fan**, **Galen Suppes** and **Fu-hung Hsieh**, University of Missouri-Columbia
- 74 Towards Characterizing the Active Coagulation Agent in *Opuntia* Spp. **Sarah M. Miller** and **Julie B. Zimmerman**, Yale University
- 75 Glycerin Carbonate—a Unique and Versatile Chemical. **Mark L. Posey**, **Haibo Zhao** and **Vincent Zhang**, Huntsman Corporation
- 76 Gold Compounds with Tripodal Bis(imidazole) Thioether Ligands as Oxidation Catalysts. **Reema Anis**, **Fangwei Liu**, **Eunmi Hwang** and **Maria Contel**, Brooklyn College and the Graduate Center, The City University of New York
- 77 New Water Soluble Gold(I) Compounds and Their Application in C-C Coupling Reactions. **Benelita T. Elie**, **Tasmin Chowdhury** and **Maria Contel**, Brooklyn College and the Graduate Center, The City University of New York
- 78 Copper-Catalyzed Synthesis of Oxazolidinones Via Four-Component Coupling Between Aldehydes, Amines, Alkynes, and Carbon Dioxide. **Woo-Jin Yoo** and **Chao-Jun Li**, McGill University
- 79 Properties That Stabilize Proteins to Enzymatic Attack. **Li Zhuo** and **Justin R. Barone**, Virginia Tech
- 83 Water Purification Using Simplified Solar Distillation Process. **Mohammad Musaddaq¹**, **Shyam Shukla¹**, **Alka Shukla²** and **Kenneth Dorris¹**, (1)Lamar University, (2) Southeast College
- 84 Synthesis of a Coordinated Ionic Liquid-(C₄H₉)₄NBr•C₆H₁₁NO. **Dishun Zhao**, **Xiaolei Bao** and **Tong Wu**, Hebei University of Science and Technology
- 85 Green Gates to Solid Waste Mangement in a Chemistry Laboratory. **S. Bhanumati**, Reader
- 86 Comparison of “Green” Concentrate and Ready-to-Use Products. **George R. Thompson**, Chemical Compliance Systems, Inc., **Chuck A. Hodge**, Ecolab Research Center and **Cayce Warf**, Ecolab
- 87 Web-Based Systems That Provide Triple Bottom Line Accounting. **George R. Thompson**, Chemical Compliance Systems, Inc.
- 88 Green Engineering and Zero Emission: New Strategies for ISO 14001 Environmental Management System. **Omid Tavakoli**, Osaka Prefecture University
- 89 Analysis of the Environmental Impact of Phenol Wastewater Treatment Processes. **Enrique A. Campanella**, Instituto de Desarrollo Tecnológico para la Industria Química (UNL—CONICET) and **Guillermo A. Ontiveros**, Universidad Nacional del Litoral

PROCESS DESIGN

- 90 Alcohol Cross-Coupling Reactions Catalyzed by Ru and Ir Terpyridine Complexes. **Dinakar Gnanamgari**, Yale University
- 91 Environmentally Friendly Approach to Microwave-Assisted Organic Synthesis of Imidazo[1,5-a]Pyridines. **Anastasia S. Lyons**, Clark Atlanta University—USDA/Forest Services/Forest Products Laboratory, **Roger M. Rowell**, University of Wisconsin and **Xiu Ren Bu**, Clark Atlanta University

SOLVENTS AND SOLVENT SYSTEMS

- 92 The Development and Application of Room Temperature Ionic Liquids. **Xiaomei Hu**, Aston University

SYNTHESIS

- 93 2008 HANCOCK AWARD RECIPIENT High-Throughput, Low-Waste Synthesis of Well-Defined Gold Nanoparticles In Microcapillary Flow Reactors. **Lallie McKenzie** and **James Hutchinson**, University of Oregon
- 94 Photo-Induced Solid State Absolute Asymmetric Synthesis In Nanocrystalline Suspensions. **Farnosh Family** and **Miguel Garcia-Garibay**, University of California
- 95 Purification Strategies Via Greener Methods for Reductive Amination Reactions Using Resin-Bound Agents. **Hephzibah J. Kumpaty**, University of Wisconsin—Whitewater

ENVIRONMENTAL DECISION MAKING AND METRICS

- 80 Diesel Engine Exhaust and Endocrine Disruption. **Leo Petrilli**, Private Citizen
- 81 Synthesis of Highly Fluorescent Gold Nanoparticles for Sensing Mercury(II). **Huan-Tsung Chang** and **Chih-Ching Huang**, National Taiwan University
- 82 Environmental Impact of the Two Process for Pseudoboehmite Obtention Using GCES Software. **Gabriel Camargo¹**, **Juan Carlos Moreno¹**, **Juliana Serna¹**, **Joaquin Tirano¹** and **Hugo Martin Galindo²**, (1)Universidad de los Andes, (2)Universidad Nacional de Colombia

- 96 Using a Capillary-Based Microreactor Screening System in Green Analytical Chemistry: Throughput Study. **Lei Hong** and Stephen Weber, University of Pittsburgh
- 97 Chitosan Based Scaffolds by Lyophilization and *sc* CO₂ Assisted Methods for Tissue Engineering Applications: A Benign Green Chemistry Approach. **Kumari Rinki** and Pradip Kumar Dutta, Motilal Nehru National Institute of Technology, Allahabad
- 98 Synthesis of Some New Bispyrrolidine Derivatives for Biological Interest. **Amal Sabet Yanni**, Assiut University
- 99 A Mild and Environmentally Friendly α -Bromination of Ketones in Ionic Liquid Using 1,3-Dibromo-5,5-Dimethylhydantoin (DBDMH) and UHP in H₂O. **Soon-Uk Chang** and Jong Chan Lee, Chung-Ang University
- 100 A New Method for Oxidation of Benzylic Alcohols Using MgBr₂/UHP in Ionic Liquid. **Hee Joong Park** and Jong Chan Lee, Chung-Ang University
- 101 Simple and Efficient Oxidation and α -Bromination of Benzylic Alcohols by Using Br₂/UHP in Ionic Liquid. **Jimi Kim** and Jong Chan Lee, Chung-Ang University
- 102 New Method for α -Bromination of Ketones Using Br₂ and β -Cyclodextrin in H₂O. **Seul Lee**, Chung-Ang University and Jong Chan Lee, Chung-Ang University
- 103 New Method for Oxidation of Benzyl Alcohols Using Ionic Liquid. **Seungbae Lee** and Jong Chan Lee, Chung-Ang University
- 104 Fluorinated Polymeric Binap Ligand for Asymmetric Hydrogenation in *sc* CO₂. **Ozlem Erdem** and Bilgehan Guzel, CU Science and Letters
- 176 2008 Breen Fellowship Recipient: Biocatalytic Approaches to the Asymmetric Oxidation of Sulfides and Alkenes. **Antonio Osorio-Lozada** and Horacio F. Olivo, The University of Iowa.
- 177 2008 Hancock Award Recipient: Utilization of Linear-Dendritic Copolymers as Aqueous Nano-Reactors for Greener Cycloaddition, Oxidation and Polymerization Syntheses. **Arsen Simonyan** and Ivan Gitsov, State University of New York, Syracuse, NY.

EDUCATION AND OUTREACH

- 105 2008 Breen Fellowship Recipient: Integration of Green Chemistry Experiments In Chemistry Teaching Methods Course. **Mageswary Karpudewan**, Zurida Hj Ismail and Norita Mohamed, University Sains Malaysia



- 106 Greening the Undergraduate Organic Chemistry Laboratory through the Biginelli Reaction. **Lois Ablin**, Oral Roberts University
- 107 Project Green at the University of Pittsburgh. **Lawrence B. Friedman**, University of Pittsburgh
- 108 The Role of Guided Inquiry and Microscale Chemistry in Green Chemistry. **Alka Shukla¹**, Shyam S. Shukla², Mohammad Musaddaq², Leena Purohit³ and D. Shukla⁴, (1)Southeast College, (2)Lamar University, (3)Asish Higher Secondary School, (4)MNS BED College
- 109 Greening up the Synthesis of Aspirin. **Kathleen D. Field** and Carolyn Supplee, Monmouth University

ENVIRONMENTAL DECISION MAKING AND METRICS

2:00 PM – 5:40 PM

Applications and Tools for Environmental Decision Making

SOUTH AMERICAN AB (CAPITAL HILTON)

SESSION CHAIR: Richard Helling, The Dow Chemical Company

- 2:00** 110 LCA and EHS Comparison of Biocatalytic and Chemical Pharmaceutical Synthesis: 7-ACA. **Concepción Jiménez-González¹**, Richard K. Henderson¹, David JC Constable¹, Chris Preston¹ and John Woodley², (1)GlaxoSmithKline, (2)Technical University of Denmark
- 2:40** 111 Natural Oil Polythiols and Polyols—a Life Cycle Comparison. **Thomas A. Upshaw**, William J. Fisher and Eric J. Netemeyer, Chevron Phillips Chemical Co LP
- 3:00** 112 Clean and Green: Progress in the Development of Environmentally-Friendly Lubricants. **Alan C. Eachus**, Independent Consultant
- 3:20** Break
- 3:40** 113 Automated Ammunition Design for Demil Utilizing Web-Based “Green” Capabilities. **George R. Thompson¹**, Kevin Kennedy¹ and Tyrone D. Nordquist², (1)Chemical Compliance Systems, Inc., (2)U.S. Army Defense Ammunition Center
- 4:00** 114 Sustainability Framework for Process and Product Development. **Carol English**, Cytec Industries Inc, David Taschler, Air Products & Chemicals, Inc. and Charlene A. Wall, BASF Corporation
- 4:20** 115 CleanGredientsSM as a Consensus-Based Tool. **Alec Gosse** and Topher Buck, GreenBlue
- 4:40** 116 Chemical Product Evaluation and Screening—Tools for Real World Decision Making. **Marilyn Johnson**, Dolphin Software, Inc.

CATALYSIS

2:00 PM – 5:40 PM

Catalysis: Session I

FEDERAL ROOM A (CAPITAL HILTON)

SESSION CHAIR: Milton R. Smith III, Michigan State University

Technical Program, *Continued*

- 2:00** 118 Siliceous Mesocellular Foam (MCF) Supported Catalysts for Green Chemistry. **Jaehong Lim**, Su Seong Lee and Jackie Y. Ying, Institute of Bioengineering and Nanotechnology
- 2:20** 119 The Use of Transparent Colloidal Titania Sol for Degradation of MTBE and Nitrophenol. **Shyam S. Shukla¹**, Kenneth Dorris¹, Hardik Shah¹, Mohammad Musaddaq¹ and Richa Shukla², (1)Lamar University, (2)University of Texas Medical Branch
- 2:40** 120 Multifunctional Binary METAL Oxide Composite Nanostructures. **Alex Ibadon**, Gilian Greenway and Yue Yue, University of Hull
- 3:00** Break
- 3:20** 121 Adsorption and Reaction of Multifunctional Oxygenates on Transition Metal Surfaces. **J. Will Medlin**, University of Colorado
- 3:40** 122 Development of An Enzymatic Process for Lipitor. **Michael P. Burns**, David W. Bauer, Alastair Denholm, Aoife Fahy, Cathal Healy, John O'Shaughnessy, Éanna O'Maitiú, Floriana Stomeo, Gillian Whittaker and John W. Wong, Pfizer
- 4:00** 123 Biocatalytically Synthesized Polypyrrole. **Ramaswamy Nagarajan¹**, **Rahul Garhwal¹**, Subhalakshmi Nagarajan¹, Jayant Kumar¹, Ferdinando F. Bruno² and Lynne A. Samuelson², (1)University of Massachusetts Lowell, (2) U.S. Army RDECOM Natick Soldier Center
- 4:20** 124 Biocatalytic Production of Unnatural Cyclic Secondary Amino Acids for Peptidomimetic Pharmaceuticals. **John Grate**, Codexis, Inc.
- 4:40** 126 Asymmetric Aldol Reaction Between Benzaldehyde and 2-Butanone in Coordinated Ionic Liquids. **Dishun Zhao¹**, Hongyan Cui¹, Erhong Duan² and Qian Li¹, (1)Hebei University of Science and Technology, (2)Tianjin University

INVITED PAPERS

2:00 PM – 2:40 PM

Natural Capitalism

FEDERAL ROOM B (CAPITAL HILTON)

SESSION CHAIR: Bob Peoples, ACS Green Chemistry Institute

- 2:00** 127 Natural Capitalism. **Stuart A. Jones**, Interface Americas, Inc.

2:40 PM – 3:10 PM

KeLa Energy Clean Coal Technology

FEDERAL ROOM B (CAPITAL HILTON)

SESSION CHAIR: Bob Peoples, ACS Green Chemistry Institute

- 2:40** 178 KeLa Energy Clean Coal Technology. **Larry Moot**, KeLa Energy LLC

SYNTHESIS

2:00 PM – 3:40 PM

Synthetic Processes

NEW YORK (CAPITAL HILTON)

SESSION CHAIR: Janet Nelson, Biotechnology Industry Organization

- 2:00** 128 Convergent Green Synthesis of Linezolid (Zyvox). **William R. Perrault**, James B. Keeler, William C. Snyder, Christian L. Clark, Michael R. Reeder, Richard J. Imbordino, Rebecca M. Anderson, Nabil Ghazal, Stephen L. Seacrest and Bruce A. Pearlman, Pfizer
- 2:20** 129 A Practical and Green Chemical Approach for the Manufacture of NK1 Antagonist LY686017. **Michael E. Kopach**, Tony Zhang, Scott Coffey, Alfio Borghese, Michael Kobierski and William Trankle, Eli Lilly and Company
- 2:40** 130 Synthesis of Amino Functionalised 2,4,6-Triarylpyridines and 1,5-Diketones Via Process Intensification on Rotating Surfaces. **Nicole M. Smith**, Marck Norret and Colin L. Raston, University of Western Australia
- 3:00** 131 The Synthesis of the Hollow Titanium Silicate Zeolite(HTS) and Its Application in Catalysis. **Min Lin**, Bin Zhu, Xingtian Shu and Xieqing Wang, Research institute of Petroleum Processing, SINOPEC

PROCESS DESIGN

3:40 PM – 5:40 PM

Fine Chemical Process Design

NEW YORK (CAPITAL HILTON)

SESSION CHAIR: Julie Manley, ACS Green Chemistry Institute Pharmaceutical Roundtable

- 3:40** 132 Solvent and Copper Free Sonogashira Reactions Utilizing High-Speed Ball Milling. **Dennis A. Fulmer**, University of Cincinnati
- 4:00** 133 A Collaborative Partnership to Develop Strategies for Waste Minimization and Solvent Recovery for the Celecoxib Process. **Mariano J. Savelski¹**, C. Stewart Slater¹, Gregory Hounsell², Daniel Pilipauskas² and Frank Urbanski², (1)Rowan University, (2)Pfizer, Inc.
- 4:20** 134 Palladium Removal from Reaction Mixtures by Fixed Bed Adsorption. **Michael J. Girgis¹**, Laura E. Kuczynski², Sonia M. Berberena², Caitlin A. Boyd², Pamela L. Kubinski², Megerle L. Scherholz², Donald Drinkwater¹, Min Yang¹, Xiaoxuan Shen¹, Stan Babiak¹, Stephanie Farrell², Robert Hesketh² and Brian G. Lefebvre², (1)Novartis Pharmaceuticals Corporation, (2)Rowan University
- 4:40** 135 Process Improvement of a Crystallization Using a Green Engineering Approach. **Daniel Sujo N.¹**, Stephanie Farrell² and Robert P. Hesketh², (1)Siegfried (USA), Inc., (2)Rowan University
- 5:00** 136 Developments toward a Green Stille Reaction. **Nicole M. Torres¹**, William P. Gallagher² and Robert E. Maleczka Jr.¹, (1)Michigan State University, (2)Bristol-Myers Squibb Company

Wednesday Evening

6:00 PM – 6:45 PM

Reception

CONGRESSIONAL ROOM & CAPITAL TERRACE (CAPITAL HILTON)



6:45 PM – 9:00 PM

BANQUET SPEAKER: Jonathan Lash

President, World Resources Institute
PRESIDENTIAL BALLROOM (CAPITAL HILTON)

Thursday, June 26, 2008

Thursday Morning

7:00 AM – 8:00 AM

Continental Breakfast

UPPER LOBBY (CAPITAL HILTON)

7:00 AM – 3:30 PM

Registration

FOYER 1 (CAPITAL HILTON)

8:00 AM – 8:10 AM

Opening Remarks/Student Poster Awards

PRESIDENTIAL BALLROOM (CAPITAL HILTON)



8:10 AM – 9:00 AM

KEYNOTE ADDRESS: Steven Chu

Director, Lawrence Berkeley National Laboratory

“The Energy Problem and What We Can Do About It”

PRESIDENTIAL BALLROOM (CAPITAL HILTON)

9:00 AM – 9:30 AM

Tea and Coffee Break

UPPER LOBBY (CAPITAL HILTON)



CATALYSIS

9:30 AM – 12:10 PM

Catalysis: Session II

FEDERAL ROOM A (CAPITAL HILTON)

SESSION CHAIR: Will Medlin, University of Colorado at Boulder

- 9:30** 137 Environmentally Attractive Metal-Catalyzed Reduction of Alkyl Halides. **Jian Yang** and Maurice Brookhart, UNC-Chapel Hill
- 9:50** 138 The Greening of the Aerobic Oxidation of *p*-Xylene to Terephthalic Acid. **Walt Partenheimer**, Consultant, DuPont (retired)
- 10:10** 140 Highly Efficient Copper Mediated Atom Transfer Radical Addition (ATRA) in the Presence of Reducing Agents. **Tomislav Pintauer**, Duquesne University
- 10:30** 141 Novel Metal Oxide Catalysts and Process for Methacrylic Acid Production Using Isobutane as the Feedstock. **Manhua Mandy Lin** and Krishnan Pillai, EverNu Technology LLC
- 10:50** 142 Catalytic Reforming of *n*-Heptane on Platinum-Zinc Supported on Gamma-Alumina. **Mehdi Vadi**, Islamic Azad University Fasa Branch and Hamid Daneshvar, Islamic Azad University Firozabad Branch
- 11:10** 143 Catalytic Reforming of *n*-Heptane on Platinum-Copper Supported on Gamma-Alumina. **Mehdi Vadi**, Islamic Azad University Fasa Branch and M. Mozafare, Islamic Azad University Firozabad Branch
- 11:30** 144 Catalytic Reforming of *n*-Heptane on Platinum-Rhenium Supported on Gamma-Alumina. **Marjan Bazargane**, Islamic Azad University Firozabad Branch and Mehdi Vadi, Islamic Azad University Fasa Branch

NEW MATERIALS

9:30 AM – 12:10 PM

New Materials: Session I

SOUTH AMERICAN AB (CAPITAL HILTON)

- 9:30** Welcoming Remarks.
- 9:35** 145 Ecomate—Environmentally Benign Foam Blowing Agent. **John A. Murphy** and John F. Timberlake, Foam Supplies Inc.
- 9:55** 146 Future Designs of Pressure Sensitive Adhesives. **Steven J. Severtson**, University of Minnesota, Carl Houtman, USDA, Forest Products Laboratory and Larry Gwin, Franklin International
- 10:15** 147 Powder Coatings Based on Seed Oils. **Jim D. Earls**, Fabio Aguirre, Maurice J. Marks and Jerry E. White, The Dow Chemical Company
- 10:35** 148 Photo Polymer Systems for Environmentally Benign Preparation of Films and Coatings. **Emily Stoler** and John C. Warner, Warner Babcock Institute for Green Chemistry

Technical Program, *Continued*

- 10:55** 149 Synthesis and Properties of a New Seed Oil-Based Thermoplastic. **Jerry E. White**, Jim D. Earls, John W. Sherman, Leonardo C. Lopez and Marvin L. Dettloff, The Dow Chemical Company
- 11:15** 150 New Value-Added Materials from Ethanol by-Products. **George E. Inglett**, S. Kim, J. Xu, D. Stevenson, D. Chen and S. Liu, USDA-ARS-NCAUR

EDUCATION AND OUTREACH

9:30 AM – 12:10 PM

Education and Outreach: Session III

FEDERAL ROOM B (CAPITAL HILTON)

SESSION CHAIR: Linda Vanasupa, California Polytechnic State University

- 9:30** 151 Integrating Green Engineering Concepts across Disciplines. **Sean P. McGinnis**, Virginia Tech
- 9:50** 152 Making It Easier to Be Green—a Green Online Curriculum Free to the World. Terrence Collins and **Chip Walter**, Carnegie Mellon University
- 10:10** 153 Beyond Green Engineering: Fostering the Ethic That Powers the Action. **Linda Vanasupa**, William Hughes and Trevor Harding, California Polytechnic State University
- 10:30** 154 Learning Materials and Teaching Strategies for Sustainability Integration in Engineering Education. **Qiong Zhang**¹, Julie Zimmerman², James R. Mihelcic¹ and Linda Vanasupa³, (1)Michigan Technological University, (2)Yale University, (3)California Polytechnic State University
- 10:50** 155 Building the Capacity of Green Chemistry Educators. **Julie Haack** and James E. Hutchison, University of Oregon
- 11:10** 156 Students Game to Learn about Green Supply Chains. **Jacqueline A. Isaacs**, Northeastern University
- 11:30** 157 Connecting Industry to K-12 Education through Green Chemistry. **Rachel Pokrandt**, Beyond Benign

11:50 PM – 1:30 PM

Lunch Break (on your own)

Thursday Afternoon

CATALYSIS

1:30 PM – 3:30 PM

Catalysis: Session III

FEDERAL ROOM A (CAPITAL HILTON)

SESSION CHAIR: John Regalbuto, National Science Foundation

- 1:30** 160 Improved Immobilization of Chiral Bisoxazolines on Silica: Application to Circulating Flow-Type Pack Bed Reactor. **SuSeong Lee**, Jaehong Lim and Jackie Y. Ying, Institute of Bioengineering and Nanotechnology

- 1:50** 159 TOF-MS Investigations on Direct Dehydroaromatization of Methane Hydrate Under Supersonic Jet Expansion Condition. **Bingsi Liu**¹, Ling Li², Xiaohong Zhao¹, C.T. Au³ and Allan S. -C. Cheung², (1)Tianjin University, (2)The University of Hong Kong, (3)Hong Kong Baptist University
- 1:50** 158 Gas Phase Conversion of Sugar/sugar Alcohol to Valuable C3 Chemicals. **Wei Yan**, Ali Tekeei, Joshua M. Ronco and Galen J. Suppes, University of Missouri-Columbia
- 2:10** 161 Catalytic Borylation for Efficient Elaboration of Aromatic Compounds. Ghayoor A. Chotana, Venkata A. Kallepalli, Anna M. Norberg, Luis A. Sanchez, Britt A. Vanchura, Robert E. Maleczka Jr. and **Milton R. Smith III**, Michigan State University
- 2:30** 162 Decarboxylative Coupling of Aromatic Carboxylic Acids with Aryl Iodides and Unfunctionalized Arenes. **Adelina M. Voutchkova**, Abigail Coplin and Robert Crabtree, Yale University

NEW MATERIALS

1:30 PM – 3:30 PM

New Materials: Session II

SOUTH AMERICAN AB (CAPITAL HILTON)

- 1:30** 164 Phase Behavior and Rheological Analysis of Cellulose Nanocrystal Aqueous Suspensions. **Esteban E. Ureña-Benavides** and Christopher L. Kitchens, Clemson University
- 1:50** 165 “Green” and Size-Controlled Synthesis and Seed-Mediated Growth of Pd Nanoparticles. **Juncheng Liu** and Christopher B. Roberts, Auburn University
- 2:10** 166 Synthesis of Nanophase Mn(VII) Oxide Using Green Technology and Its Applications. **R. K. Vempati**, Southern Methodist University, Gajanan Bhat, University of Tennessee at Knoxville and Richard Wagner, PhycoBiologics, Inc.
- 2:30** 167 Expanding the Horizons of Green Battery and Capacitor Chemistries with Nano-Porous Carbon. **Bryan D. Sawyer** and Galen Suppes, University of Missouri-Columbia
- 2:50** 168 Novel Green Chemistries to Extend Automobile Catalytic Converter Useful Life While Reducing Exhaust Gaseous Emissions. **Ewa Bardasz**, The Lubrizol Corporation
- 3:10** 169 Polymer-Filled Composite Membranes. **Xiangwu Zhang**, North Carolina State University

EDUCATION AND OUTREACH

1:30 PM – 3:30 PM

Education and Outreach: Session IV

FEDERAL ROOM B (CAPITAL HILTON)

SESSION CHAIR: Linda Vanasupa, California Polytechnic State University

- 1:30** 170 Providing Real-Life Experience While Learning Green Chemistry Principles. **Dalila G. Kovacs**, Grand Valley State University

- 1:50** 171 Towards the Greening of Our Minds: A New Course Offered at Washington College, Chestertown, MD. Anne E. Marteel-Parrish, Washington College
- 2:10** 172 Teaching Students about Consumer Exposure to Hazardous Chemicals. Shonali Laha, Florida International University
- 2:30** 173 Using the Rowan University Engineering Clinic Model to Implement Green Engineering Partnerships with the Pharmaceutical Industry. C. Stewart Slater, Mariano J. Savelski, Brian G. Lefebvre, Stephanie Farrell and Robert P. Hesketh, Rowan University
- 2:50** 174 Understanding and Implementing the Principles of Green Chemistry in Industry. Amy S. Cannon, Beyond Benign: A Warner Babcock Foundation
- 3:10** 175 C2B2—a Biorefining Collaboratory. John R. Dorgan¹, Alan Weimer², Ryan T. Gill², Will Medlin², Kenneth F. Reardon³ and Al Darzins⁴, (1)Colorado School of Mines, (2)University of Colorado at Boulder, (3)Colorado State University, (4)National Renewable Energy Laboratory

3:30 PM – 4:00 PM

Tea and Coffee Break/Closing Session

SESSION CHAIR: Bob Peoples, ACS Green Chemistry Institute
PRESIDENTIAL BALLROOM (CAPITAL HILTON)



Notes

Notes



Abstracts

1. A Green Chemistry Assessment for Analytical and Chemical Processes

Julee Driver¹, Douglas Raynie¹ and Paul Jackson², (1)South Dakota State University, Brookings, SD, (2)St. Olaf College, Northfield, MN

The 12 Principles of Green Chemistry are used to guide the development of a straightforward, yet thorough method to assess and compare analytical or chemical processes for their health and environmental impact. Similar assessments may neglect one or more of the major concepts in the 12 Principles. For example, a “green analytical profile” has been developed in concert with the National Environmental Methods Index database (www.nemi.gov) and neglects energy considerations. Our proposed assessment, rates analytical methods against waste amount and type, chemical health and environmental hazard, and energy requirements. Reagents, procedures, and instrumentation are evaluated. Metrics were developed to calculate waste amount and energy use. During the calculation of waste, relative waste generated and sample size are considered. The energy-use metric assists in placing a value on the energy requirements of instrumental methods. The overall rating in each category can be easily fit into a visual presentation to allow for an at-a-glance comparison of several methods.

2. Instructional Resources for the Teaching of Green Analytical Chemistry

Douglas Raynie, South Dakota State University, Brookings, SD

The development of instructional materials for including green chemistry into the analytical curriculum trails the development of similar materials for other chemical disciplines. The revision of a popular analytical laboratory manual provided an opportunity to work green chemistry into the curriculum. A chapter on green analytical chemistry was written and focuses on what are considered green methods, how to assess the “greenness” of an analytical procedure, and engage student thought-processes toward analytical problem solving in a green manner. For each experiment, a “green perspective” is included to present a green profile (using the profile developed for the National Environmental

Methods Index, www.nemi.gov) of the experiment and address questions on how to make the experiment more green. In this presentation, this laboratory manual and the developments toward green chemistry are presented.

3. Micro-Scale HPLC Generates < 1% of the Solvent Waste of Conventional Analytical LC

Justin E. Kittell, Phil Paul, Don Arnold, Dave Neyer, Phil DeLand and Jason Rehm, Eksigent Technologies, Dublin, CA

HPLC is a nearly universal analytical technique applied on a routine basis around the world for separation, quantitation and identification of chemical compounds by industry and academia. Approximately 130,000 conventional HPLC instruments are in use today, with another 15,000 instruments sold yearly. The majority of these instruments use a typical column diameter of 4.6 mm internal diameter (I.D.) with most analytical methods using a flow rate of 1 ml/min. If the typical HPLC is used 20 hours a week, a single conventional HPLC would require 60 L of solvent to operate and generate 60 L of mixed organic/aqueous waste per year. This translates into 8 million liters of solvent produced each year to supply mobile phase for analytical HPLC while producing the equivalent of nearly 40,000 55-gallon drums of mixed waste that must be disposed of per year.

Micro-flow HPLC, that is, liquid chromatography performed with small I.D. chromatography columns, typically 0.3 mm, and low flow rates (4 μ l/min), provides a significant savings in solvent usage and mixed waste generation over conventional HPLC. Wide-scale use of micro-flow HPLC would reduce toxic waste generated by chemical researchers in academia and industry by millions of liters per year. By using a 0.3 mm I.D. column on a micro-flow HPLC and reducing the flow rate to 4.3 μ l/min so that the linear velocity of the mobile phase through the column is equivalent to a conventional HPLC, a mobile phase volume savings of greater than 99% is realized. Any HPLC method that has been validated and developed over the past decades can be directly transferred to micro-flow HPLC by scaling only column I.D., flow rate, and sample volume, yielding the same separation, sensitivity and retention times, but with a significant savings in solvent usage and mixed waste generation.

Abstracts, *Continued*

4. Direct Analysis in Real Time (DART)/ High Resolution Mass Spectrometry: Green Chemistry Applications

Ted H. E. Mendum and John C. Warner, Warner Babcock Institute for Green Chemistry, Woburn, MA

Direct Analysis in Real Time (DART) is a recently introduced sample introduction technique for mass spectroscopy which is performed in the open atmosphere and requires no sample preparation. When coupled with a high-resolution high-accuracy mass spectrometer, identification of the composition of mixtures is especially facile. This technology is often used for the analysis of finished products. The potential for Green Chemistry is in the identification of toxic or harmful reaction byproducts at low but significant levels EARLY in the synthetic process. Including this type of analysis at a time when scale-up and eventual production are still being designed, when it is cheaper and simpler to adjust reaction conditions and purification steps, allows for a more sustainable outcome.

5. Green Product Design of Temperature Sensors

Maria Nydia Ruiz Felix, Robert P. Hesketh, Robert Newland and Dariusz Kuciauskas, Rowan University, Glassboro, NJ

Considerable interest has focused on the design of new products that identify processes, ingredients and systems that are environmental friendly. Chemical products can be manufactured by following different routes. Every route has a planning, research and development cycle. Because of their simple design and low cost, irreversible thermochromic sensors can be used in many applications in the food, textile, and commercial product industries. Initially thermochromic sensors appear white, when the specific temperature is reached, the sensor color changes. This indicates that the substance the sensor was placed on reached the temperature of activation.

Commercial sensors and Rowan sensors were tested using several methods. Parameters such as activation temperatures, activation time, amount of thermochromic mixture in the sensor, mixture quality, and particle size were taken into consideration. The labels were produced and characterized in a temperature range of 61°C to 97°C and 106°C to 131°C. The performance characteristics of Rowan's sensors are similar to the ones currently on the market.

6. Rapid Evaluation and Functional Design of SMB Chromatography for Separation of Vegetable Oil-Derived Hydroxy Methyl Esters

Shawn D. Feist, Bruce W. Pynnonen, Timothy C. Frank and Zenon Lysenko, The Dow Chemical Company, Midland, MI

Simulated Moving Bed (SMB) processes have become the industry standard for many production-scale separation applications, and the technology continues to receive heightened attention in the fields of pharmaceuticals, bio-separations, and enantiomeric separations. Advances in the technology have also made it a very viable, cost-effective option for low relative volatility, heat-sensitive specialty materials that cannot be separated via traditional means such as distillation or evaporation. The Dow Chemical Company has developed process technology involving methanolysis, hydroformylation, and hydrogenation of vegetable oils to produce hydroxyl methyl esters as precursors to polyurethane and other value-adding products. Although the hydroformylation/hydrogenation reaction mixture can be used without separation to produce polyols suitable for flexible polyurethane foams, production of other specialty products such as rigid foams and cast parts requires isolation of various fractions rich in monols or diols or low in non-hydroxy components. To fully obtain maximum value from bio-based resources in the specialty product realm, a means of separating the various reaction components is needed. In this work, a simulated moving bed (SMB) chromatography miniplant was used to determine the viability of the technology for separating these components. The technology was shown to be a viable option for 1) separating a soy reaction mixture into a fraction with 95%

monol and another with > 99% diol; 2) separating a soy reaction mixture with saturates removed into two fractions with > 95% monol and > 99% diol. All purities are on a monol/diol only basis.

7. Fractionation of Lignocellulosic Biomass Feedstocks

Lisette Ngo Tenlep, South Dakota State University, Brookings, SD and Doug Raynie, South Dakota State University

Lignocellulosic biomass has long been recognized as a potential low-cost source of mixed sugars for fermentation to fuel ethanol. The low rate at which biomass is converted to sugars and the coproduction of fermentation inhibitors result in pretreatment strategies to prepare the biomass for subsequent biological conversion to biofuel. New approaches for designing improved energy feedstocks, deconstructing plant cell walls, and transforming their polysaccharides to fermentable sugars are needed. Distillers dried grains with solubles (DDGS), the residue from current ethanol production, and switchgrass were selected as biomass feedstocks. Heating was by way of convection and the biomass samples were hydrolyzed at 140°C for 20 minutes with a mixture of dilute sulfuric acid, ethanol and methyl isobutyl ketone, mimicking the NREL (National Renewable Energy Laboratory) clean fractionation procedure. The resulting extracts comprised an aqueous layer and an organic layer. The layers were separated and analyzed with HPLC for determination of sugars, byproducts and degradation products. The biomass residues were analyzed for determination of cellulose, hemicellulose and lignin following the procedures patterned after the NREL standard analytical procedures and modified for biomaterial process streams. The aqueous layer consisted mostly of hemicellulose; the organic phase comprised lignin and the cellulose remained in the biomass residues. Mannose was the most abundant sugars in all layers, whereas glucose was the least represented sugars in all layers. Continuing studies are investigating the presence of single sugars, cellulose, hemicellulose, and lignin in biomass residues.

8. System for Bioremediation of Effluents

John R. Roheim, NCH Corporation, Irving, TX

Naturally occurring microorganisms have been utilized for many years to facilitate the bioremediation process of municipal, industrial and agricultural wastewaters. Historically, bacteria have only been available commercially as dormant spores and at relatively low activity levels. These limitations have made the use of bacteria economically prohibitive for many systems to utilize the appropriate high levels of bacteria required to significantly reduce Biochemical Oxygen Demand (BOD) and Fats, Oils and Greases (FOGs). Extensive biochemical and equipment research has resulted in the development of a novel patented process which efficiently produces and dispenses live vegetative bacteria on-site every day for bioremediation of wastewaters.

The automated BioAmp® system is a cost effective, easy to operate, dosing system that dispenses high levels of a renewable feedstock, made up of naturally occurring strains of *Pseudomonas* and *Bacillus* species, directly into problematic drain lines. These bacteria release enzymes to degrade organic matter in drain lines, which is then converted by natural biochemical reactions into carbon dioxide and water. The BioAmp delivers the equivalent of 25–50 lbs. of commercially available dry bacterial powdered product every 24 hours, while eliminating drum storage and disposal concerns. This is accomplished at a cost of less than 10% of comparable quantities of dry powdered bacteria and saves energy by producing product on-site and reducing the consumption of large amounts of energy required for manufacturing and shipping. In addition, the BioAmp is a greener synthetic pathway that provides a safer alternative to commonly used toxic drain maintainers, such as acid, caustic, and solvents. With this new technology, efficacy data has been generated in a number of case studies to demonstrate reproducible BOD reduction. The use of this VOC-free, bio-based technology has proven successful in several industries, including food processing and petroleum refining, and is currently being researched for applications in additional industries.

9. Liquid Carbon Dioxide-Based Production of Leather

Doug Raynie, South Dakota State University and Jeremy Kroon, South Dakota State University, Brookings, SD

The purpose of this project is to develop a liquid carbon dioxide-based process for the manufacturing of leather. Current practices use large amounts of water as the solvent leading to excessive amounts of wastewater. The cleanup of this wastewater generates the largest cost for the leather producers. In addition because the water diffuses very slowly, the tanning process is quite lengthy. Carbon dioxide thus has several advantages as a solvent over the traditional water solvent. It has higher diffusivities than water and should allow for faster leather production with less waste.

Using liquid carbon dioxide for waterproofing and dyeing of leather show the greatest probability of success and is where the work is currently focused. Commercial waterproofing agents fall into five classes: fluorocarbons, silicones, waxes, aqueous-based oils, and fluoropolymers. Work thus far has shown that examples from each of these classes are soluble in super-critical carbon dioxide. The agents are still being investigated to determine their solubility in liquid carbon dioxide. The sorption of these substances onto leather is also being examined. This will relate to future work where liquid carbon dioxide may potentially be used in the degreasing, retanning, deliming and tanning steps of leather production

11. "Green" Comparisons for Functionally Equivalent Products in Federal Supply Catalogs

George R. Thompson, Chemical Compliance Systems, Inc., Lake Hopatcong, NJ and Raymond Paulson, Fleet Readiness Center Southwest North Island, San Diego, CA

Federal agencies must preferentially purchase environmentally preferable, or "green," products, as required by Executive Order (EO) 13423. This EO requires federal agencies to acquire goods and services that include consideration of environmentally preferable products, renewable materials (bio-based and recycled containing), energy and water efficiency. GSA and DLA have included only minimal, chemical-specific criteria in their definitions of "green" chemical products for them to be so listed in their catalogs. EPA has named 33 end point criteria for environmentally preferable products. The U. S. Navy utilized the Web-based "Green" Product Compliance Analytical System (GP-CAS), from Chemical Compliance Systems, Inc. (CCS), that incorporates 43 ecological, health, and safety endpoint criteria, including the EPA 33 end point criteria for environmentally preferable products, to compare the "greenness" of individual chemical products listed within five separate National Stock Numbers (NSNs). (Each NSN includes functionally equivalent products available from various manufacturers.) These five NSNs each contained 3–10 different chemical products and encompassed a spectrum of product functions—a total of 35 products were evaluated. All output reports for the 35 products were printed in less than 15 minutes. Within the five NSNs analyzed, only one (spray lacquer) was both functionally equivalent and equally "green." The other four NSNs showed "green" ranges of 11–24% and diverse regulatory impacts. We also identified a consistent inverse proportionality for "green" Grades and "MSDS Total %" of constituents identified.

This analysis demonstrates that GP-CAS readily differentiates "green" disparities within functionally equivalent NSNs and additionally identifies both unique regulatory and total regulatory impacts. GP-CAS also tallies the number of MSDS constituents and their "Total %" of the product. Together, these factors provide the user with a broad spectrum of in-depth information to facilitate product acquisition decisions and hazard assessments for federal facility executive order and regulatory compliance.

12. The Importance of Chemical Ranking Systems: A Department of Defense Study

Carole A. LeBlanc, Office of the Deputy Under Secretary of Defense, Arlington, VA

To gain insight into improving the management of emerging contaminants (ECs) within the Department of Defense (DoD), the EC Directorate (Office of the Assistant Deputy Under Secretary of Defense for Environment, Safety and Occupational Health) worked with the Air Force Institute for Operational Health to gather and evaluate information on chemical ranking and substitution systems within the Department.

The review of chemical ranking systems was part of an effort to comply with White House Executive Order (EO) 13423 to reduce the environmental, energy and transportation impacts of federal activities by using lower-risk chemicals. Chemical ranking systems developed by industry, other government agencies and non-profit organizations were also surveyed for their applicability to DoD.

Seven chemical ranking systems were selected for detailed consideration based on accessibility, cost, flexibility, database quality and potential for wider usage. While the existing systems do not meet all of the needs likely to occur within DoD, the Department's compliance with EO 13423 could well be advanced by adapting a chemical ranking system(s) to accommodate ECs, as well as known toxic and hazardous chemicals. This talk aims to inform the audience of the availability and practicability of application-specific, decision-making tools in the selection of greener chemicals, in the hope of further minimizing future environmental, health and cost impacts incurred by organizations and suffered by society at large.

13. Characterizing and Addressing Policy Barriers to Green Chemistry in the United States

Michael P. Wilson and Megan R. Schwarzman, MD, MPH, University of California, Berkeley, Berkeley, CA

This presentation will describe the key findings of the University of California Special Report, Green Chemistry in California: A Framework for Leadership in Chemicals Policy and Innovation. This report was commissioned by the California Legislature in 2004 and was released by the University of California Policy Research Center to the California Senate Environmental Quality Committee and Assembly Committee on Environmental Safety and Toxic Materials in March 2006. Dr. Wilson is the chief author of the report; he presented the reports' key findings before a hearing of the U.S. Senate Environment and Public Works Committee in August 2006.

The report proposes that long-standing weaknesses federal policy, notably the U.S. Toxic Substances Control Act (TSCA), have produced a flawed chemicals market in the U.S., and that these market conditions represent a fundamental barrier to the scientific, technical, and commercial success of green chemistry. The report concludes that (1) there is insufficient information in the market for the users of chemicals and chemical products to make informed purchasing decisions; (2) government is overly constrained in its capacity to assess chemical hazards and control those of greatest concern; and (3) these market conditions have dampened the motivation of the private sector to invest in green chemistry at a level commensurate with the pace and scale of the chemical production system. The report characterizes these barriers to green chemistry as the chemical Data Gap, Safety Gap, and Technology Gap, respectively.

The report proposes that policy developments occurring in the European Union, such as REACH, along with efforts by U.S. businesses to "clean" their supply chains of hazardous chemicals, present governments with a unique opportunity to implement a modern, comprehensive approach to chemicals policy that would favor green chemistry by correcting these flaws in the market.

Abstracts, *Continued*

14. Greenhouse Gas Emission Reduction and Trading In North America: How Can the Chemical Sector Engage?

Kellee James, Chicago Climate Exchange, Chicago, IL

Session will cover “carbon trading” from a legislative, economic and operational standpoint. Join this session to discuss pending national cap and trade legislation, how companies in the chemical sector are already participating by reducing emissions and getting involved in the emerging carbon market and how a carbon inventory, reduction, and trading platform works.

15. Characteristics and Performance of a Wood Preservative Produced from Pyrolysis Oil

Philip H. Steele, El-Barbary Hassan, Jerome E. Cooper, Christopher V. Ruhs and Leonard L. Ingram, Mississippi State University, Mississippi State, MS

Research to determine the potential for developing an alternative wood preservative system was conducted utilizing bio-oils produced from southern pine and oak clear wood and bark feed stocks. Feed stocks were pyrolyzed in an auger reactor. Both raw bio-oil and bio-oil fractions were utilized as wood preservatives. Each bio-oil treatment was diluted with methanol to 10% and 25% concentrations and subsequently impregnated into southern pine and cottonwood wafers. A proprietary polymerization method was applied to the impregnated wood to prevent bio-oil leaching. The intrinsic fungicidal activity of the bio-oils was evaluated against a brown-rot (*Gloeophyllum trabeum*) and a white-rot fungus (*Trametes versicolor*). Soil-block decay tests were conducted in accordance with accelerated soil block test described by AWWA Standard E10 to reduce the total inoculation time to approximately six weeks. Preliminary results showed that wafers impregnated with bio-oil at 25% concentration largely prevented compression strength loss. Study results indicate that the bio-oils tested have potential as a wood preservative. Researchers have hypothesized that the fungicidal activity of bio-oils may be a function of the antioxidant activity of one or more bio-oil chemicals. We tested this hypothesis by measuring the antioxidant activity of both raw bio-oils and fractions were separated by distillation from the six raw bio-oils demonstrating highest antioxidant activity.

17. Bio-Based Composites: Design for Commercialization

Richard P. Wool, University of Delaware, Newark, DE

Bio-based composite resins have been developed from plant oils (soy, canola, linseed, corn, etc) via chemical functionalization by the ACRES (Affordable Composites from Renewable Resources) group at the University of Delaware. The bio-content (C14 ratio basis) typically ranges from 50–100%. The new bio-based resin properties are comparable to petroleum based resins and their pricing is highly competitive, which is generating considerable commercial interest. The plant oil fatty acid distributions provide unique opportunities to control the molecular architecture and crosslink density. These resins are suited to composite manufacturing with natural (ligno-cellulosic, avian) or synthetic fibers (glass, carbon, kevlar) using RTM, VARTM, BMC, SMC and related liquid molding processing techniques. They form excellent nanocomposites with nanoclays, carbon nanotubes and nanocellulose. The resins can also be converted to foams via their polyols for PU foams (50% C14) or by high pressure CO₂ foaming of the liquid molding resin (85% C14). The commercial scale-up of these materials with industrial partners Cara Plastics and DynaChem Inc is discussed. The environmental impact of these new materials is significant and the nominated design for the Virgin Earth Challenge Global Warming Solutions Award is presented.

http://www.che.udel.edu/research_groups/wool/index.html
<http://www.caraplastics.com>

18. Natural Oil Polythiols and Their Utility in Polymeric Systems

Chad W. Brown, Chevron Phillips Chemical Company, LP, Bartlesville, OK

The incorporation of sulfur functionality into the backbone of polymeric systems has been known for many years as a means to provide various performance benefits such as improved adhesion and chemical resistance. One way by which sulfur is utilized in polymeric materials is through the use of polythiols as crosslinkers in thermoset systems. For instance, polythiols are known to be effective hardening agents for epoxy resins. Polythiols are also known for use with isocyanates in urethane polymers to produce polythiourethanes, although perhaps not as widely recognized. Recently interest has increased in environmentally friendly products and materials derived from renewable resources. Particular attention has been brought to raw materials derived from natural triglyceride oils, such as soybean oil. These polyolefinic materials provide a convenient route to polythiols when combined with Chevron Phillips Specialty Chemical's hydrogen sulfide (H₂S) handling and process technologies. Novel polythiols derived from soybean oil have been developed by Chevron Phillips Specialty Chemicals. The synthesis, structure, and characteristics of these polythiols will be discussed.

19. L'Oreal's Commitment to Green and Sustainable Chemistry

Michel D. Philippe, L'OREAL, Aulnay Sous Bois, France

The description of L'Oreal's Research and Development and its commitment to green and sustainable chemistry are developed. The latter is directly linked to a socially responsible business¹. L'Oreal's “green methodology” is based on the basic principles of green chemistry as defined by P. Anastas and J. Warner². To develop innovation, greater emphasis is placed on three main principles:

- the use of renewable raw materials from plants,
- the development of environmentally friendly processes,
- and the manufacture of low ecotoxicity and biodegradable ingredients.

A high percentage of ingredients used by the company are from vegetable origin. Around 40% of ingredients are sourced from renewable plants. In order to specify the potential environmental impact of these ingredients, L'Oreal assessment involves their persistence, bioaccumulation and ecotoxicity.

To select and develop eco-efficient processes, green indicators such as E-factor³ have also been introduced. Currently, the company assesses E-factors of its in-house products.

Greater emphasis is also placed on the development of new green technologies. L'Oreal has perfected an original green route to produce a new C-glycoside, Pro-Xylane, recently launched on the market⁴. The new green route is discussed in comparison with previous processes.

References: (1) www.LOREAL.com/OurCompany/SustainableDevelopment; (2) Anastas P., Warner J.C., Green Chemistry, Oxford University Press, New York, 1998, p. 30; (3) Sheldon R.A., Chem. & Ind., 1997, 12; 1992, 903; (4) Lubineau A. *et al.*, Chem. Commun., 2000, 2049-2050; Dalko M., Breton L., WO 2002051828 (L'OREAL); Philippe M., Semeria D., WO 2002051803 (L'OREAL).

20. Recent Advances in Green Chemistry Research and Development as Sources for New Eco-Friendly Materials Protection Agents

Walter Bogaerts¹, Thuy Vu Thi¹, Abdul Rauf¹, Quoc Hung Le², Hong Phong Pham², Hong Hanh Pham² and Chi Linh Do², (1)University of Leuven, Heverlee (Leuven), Belgium, (2)Vietnamese Academy of Science and Technology (VAST), Hanoi, Vietnam

Since early years of this decade the search for the availability of compounds or molecules that can potentially be derived from natural materials has been carried out. Besides from some traditional examples of such species include cashew nut oil extracts and derivatives for corrosion inhibition (e.g. in polymer coating systems), or ammorhea compounds for fouling mitigation, there is a whole "world" of other unexplored, probably more or the same efficient, compounds and species around, among which we have found 4 types of materials "Camellia sinesis" or green tea, "Nicotiana" or Tobacco, *Rhizophora* and *Mimosa* plants with their natural chemical contents and advantages that seem to fit the objectives of being used as chemical corrosion inhibitors for stainless steel, carbon steel and brass in saline, acidic and alkaline environments. Various results obtained after performing tests, both long and short terms, at room and high temperatures for green tea, tobacco and some early results for *Rhizophora* and *Mimosa* are evaluated and discussed in this paper. The new green inhibitor formulations show promise in performing as well as or better than the lab inhibitor under certain conditions.

21. Fatty Acid-Based Monomer as a Replacement for Styrene in the Production of Triglyceride-Based Polymers

Alejandrina Campanella¹, John J. La Scala² and Richard P. Wool¹, (1) University of Delaware, Newark, DE, (2)Army Research Labs, Aberdeen Proving Grounds, MD

Resins that are used to produce automobiles and many other commercial applications usually contain high concentration of reactive diluents, such as styrene, to allow the resin to be molded using resin transfer molding. Styrene is a hazardous pollutant and a volatile organic compound. Therefore, the focus of this work was to employ methacrylated lauric (MAL) acid as an alternative diluent to styrene in the production of triglyceride-based polymers. Different bio-based resins (BBR) were produced for this purpose: acrylated epoxidized soybean oil, maleinated AESO, maleinated soybean oil monoglyceride and maleinated castor oil monoglyceride. The viscosity of these resins and the mechanical properties of the bio-based polymers were analyzed. The viscosity of BBR using MAL was higher than that of BBR/styrene resins. In addition, the glass transition (T_g) of BBR/MAL polymers was in the order of 40–60°C, which were lower than the BBR/styrene polymers. Employing, ternary blends of BBR, MAL and styrene acceptable values of viscosity were obtained and the mechanical properties were improved.

22. Bioplastic Blends and Nanocomposites: New Green Materials

John R. Dorgan¹, Margaret Sobkowicz¹, Rakhi Patel¹ and Birgit Braun², (1)Colorado School of Mines, Golden, CO, (2)PolyNew Inc, Golden, CO

The now rapidly developing field of bioplastics, plastic materials based on renewable resources, provides tremendous opportunities to sustain and enhance the domestic plastics industries, the fourth largest manufacturing sector. Growth in the use of these new, greener plastics is proceeding rapidly; however, there are a number of cases in which bioplastics lack the properties needed to compete with increasingly expensive petroleum based materials. Drawing on decades of scientific knowledge about polymer blends, as well as the new emerging field of polymer nanocomposites, these property limitations can be overcome. In this lecture, the development of novel polymer

nanocomposites based on renewable cellulosic nanowhisker combined with various bioplastics is described. Time permitting, a new chemical route to novel hybridized reactively compatibilized bioplastic blends will also be described.

23. Ionic Liquids for Absorption Refrigeration

Joan F. Brennecke and Lindsay E. Ficke, University of Notre Dame, Notre Dame, IN

Ionic liquids are low melting salts that have received tremendous attention due to their potential in a wide variety of applications. One of these is absorption refrigeration. In a conventional refrigeration unit a compressor, which is the major energy requirement, is used to increase the pressure of the working fluid in the cycle. In absorption refrigeration the working fluid is absorbed into a liquid. Then a pump, which requires comparatively little energy, is used to pressurize the liquid. A heat source is needed to desorb the working fluid at high pressure. The two commercially available systems, LiBr/water and water/ammonia, have many practical disadvantages. Ionic liquids are being explored as the absorption fluid for a variety of different absorption refrigeration systems. Here we will present the necessary thermodynamic measurements, including heat capacities and heats of mixing, and calculations that show very favorable coefficients of performance compared to commercial systems.

25. Industrial Use of Ionic Liquids—Challenges and Opportunities

Peter FH Schwab¹, Matthias Seiler² and Bernd Weyershausen¹, (1)Evonik Degussa, Essen, Germany, (2)Evonik Degussa, Hanau, Germany

With this presentation we would like to change the perception that Ionic Liquids (ILs) are mainly environmentally safe or "green" alternatives to conventional organic solvents. In fact, the application potential of ionic liquids is much broader than presumed. Beyond their use as alternative solvents, ILs can be employed as process aids, e.g. in the hydrosilylation of olefins (immobilization of otherwise homogeneous catalysts) and in the specific absorption of gases. Furthermore, due to their unique properties, ILs create many interesting possibilities as performance additives and functional fluids in various materials and applications. In this context, non-imidazolium-based ILs should be of particular interest due to their availability in technical quantities and lower cost compared to their imidazolium-based counterparts. Examples of industrial applications of ILs as performance additives and functional fluids taken from Evonik Degussa's ongoing ILs research program will be presented. In addition, we will discuss the toxicology and environmental impact of the compounds, as well as challenges and opportunities in regard to the REACH legislation.

26. Water-in-Ionic Liquid Microemulsions: A New Medium for Biocatalytic Reactions

Muhammad Moniruzzaman, Noriho Kamiya and Masahiro Goto, Kyushu University, Fukuoka, Japan

Ionic liquids (ILs), representing no measurable vapor pressure, have been proven to be useful as a replacement for ordinary organic solvents to reduce volatile organic compound (VOC) emissions. However, most of hydrophilic substances such as proteins and catalysts are insoluble in most ILs. This limitation was overcome by the formation of nanometer-sized water domains in a hydrophobic IL [C₈mim][Tf₂N] (1-octyl-3-methyl imidazolium bis(trifluoromethyl sulfonyl) amide) stabilized by the layer of anionic surfactant sodium bis(2-ethyl-1-hexyl) sulfosuccinate (AOT) in the presence of 1-hexanol as a cosurfactant. The phase behavior of the AOT/water/IL system, dynamic light scattering study and solvatochromic probe study demonstrated the existence of water domains in the IL microemulsions. We tested the solubility of various enzymes and proteins in IL and in water-in-IL microemulsions. The results show that the microemulsions can solubilize enzymes and proteins, whereas IL alone or water saturated IL can not solubilize such biomacromolecules. The catalytic activity

Abstracts, *Continued*

of one of the enzymes (lipase PS) dissolved in the water domains of IL became much higher than in microemulsions of AOT in isooctane. Therefore, this work opens up new possibilities for biocatalytic reactions in ionic liquids, which are receiving increasing attention as “green” solvents for organic synthesis and catalytic processes.

27. Surface Structure and Green Chemistry in the Organic Solid State

John C. Warner and Donna Guarrera, Warner Babcock Institute for Green Chemistry, Woburn, MA

The field of noncovalent derivatization involves the design of molecular complexes [co-crystalline or eutectic] to manipulate bulk physical properties. Various structure activity relationships regarding hydrogen bonding, pi-stacking and lipophilic interactions have been established and have been demonstrated to be adequate predictors of lattice structure to physical behavior. This presentation will provide an update of recent activities exploring these structure activity relationships.

28. Comparative Assessment of Chemicals Impacts on Ecosystems and Human Health Using the USEtox Model

Olivier Jolliet¹, Michael Hauschild², Mark Huijbregts³, Manuele Margni⁴, Thomas McKone⁵, Matt MacLeod⁶, Dick Van de Meent⁷ and Ralph Rosenbaum⁴, (1)University of Michigan, Ann Arbor, MI, (2)Technical University Denmark, Lyngby, Denmark, (3)Radboud University, Nijmegen, Netherlands, (4)Ecole Polytechnique de Montreal, Montreal, QC, Canada, (5)University of California-Berkeley, Berkeley, CA, (6)Swiss Federal Institute of Technology Zuerich, Zuerich, Switzerland, (7)RIVM, Bilthoven, Netherlands

USEtox is a multimedia fate and exposure model developed to consistently compare the environmental impacts of chemicals on human health and ecosystems. Within the SETAC-UNEP Life Cycle Initiative, an international comparison of six models first enabled us to identify the crucial fate, exposure and effect issues that made models differ. A parsimonious (as simple as possible but as complex as needed) and transparent consensus model was then created within a matrix framework, containing only the most influential model elements. Covering more than 2000 substances, USEtox provides human toxicity and aquatic ecotoxicity characterization factors—a comparative measure of the impact per kg emitted substance into (urban) air, freshwater and agricultural soils. The present study applies the model to analyze the major factors affecting both human toxicity and ecotoxicity impacts, with illustrations for key chemicals. The fate part relates emission flows to masses in the environment (e.g. transport to water and residence time in water) and is common to both human- and eco-toxicity assessment, with typically 5 orders of magnitude variations between chemicals. For human toxicity, exposure factors multiply by fate to yield the intake fraction—the fraction of the emission that is taken in by the human population. Intake fractions typically range from 10⁻² for POPs and metals that bioconcentrate in the food chain down to 10⁻⁸ for the inhalation of shortly degraded VOCs. Effect measures for both human- and eco-toxicity are based on the best estimate of the hazard concentration that generates 50% of response for humans and 50% of species affected or disappeared for ecosystems. As a whole the characterization factors vary by 12 orders of magnitude for human health and 10 for ecotoxicity.

29. A Methodology for Driving Environmental Improvements in the Process Development of Active Pharmaceutical Ingredients

James A. Baird¹, Stephen Evans¹, Mark Hoyle¹, Magnus Bergqvist² and Daniel J. Horner³, (1)AstraZeneca, Macclesfield, United Kingdom, (2)AstraZeneca, Södertälje, Sweden, (3)AstraZeneca, Loughborough, United Kingdom

AstraZeneca's SHE (Safety, Health, Environment) Triggers model has been used to drive environmental improvement in the process development of Active Pharmaceutical Ingredients for a number of years. Changing industry pressures, driving new internal ways of working, led to a review of SHE Triggers to generate a fit for purpose, flexible methodology for modern pharmaceutical development.

Process development milestones are used to trigger environmental assessment tasks, with focus shifting from prevent, to minimise and render harmless through the development cycle. The methodology is driven from an early stage by a risk-based approach to the prioritisation of improvement actions, based on a simple product tonnage/material hazard model. The output is an environmental risk profile that can be easily interpreted and acted upon by process chemists and engineers, both within the company and at external contract manufacturers. Risk profiles additionally enable better resource allocation across projects, to ensure effort is focussed on the process steps with the greatest environmental impact. The risk profile is easily updated to allow re-appraisal of the process throughout the development cycle to deliver environmentally sound commercial manufacturing processes.

30. Developing Proactive Design Strategies in Nanoscience to Reduce Uncertainty, Enhance Performance and Minimize Hazard

Bettye L.S. Maddux¹, Stacey L. Harper², Robert T. Tanguay² and James E. Hutchison³, (1)Safer Nanomaterials and Nanomanufacturing Initiative, Eugene, OR, (2)Oregon State University, Corvallis, OR, (3)University of Oregon, Eugene, OR

Nanotechnology has been touted as ‘the next technological revolution,’ a revolution, however, that is already here. Nanoscale materials currently exist in over 500 manufacturer-identified nanotechnology-based consumer products currently on the market as reported by the Project on Emerging Nanotechnologies (PEN). The environmental and biological fate of these nanomaterials and their by-products is uncertain. As a result, environmental, consumer, other advocacy groups are calling for regulation and disclosure, or in some cases a moratorium of products containing nanomaterials.

In order to gain acceptance and benefit society, environmental and health considerations need to be investigated in tandem with nanomaterial synthesis. In our iterative approach, nanomaterials are designed using the principles of green chemistry, tested in biological and environmental systems and redesigned as necessary to produce nanomaterials with enhanced performance yet minimal hazard. This strategy will provide much needed data on biological impacts, improve public trust of the nanotechnology industry, and provide researchers with the information to develop safer nanomaterials.

In this presentation, we will highlight our design strategies for development of greener nanomaterials and nanomanufacturing processes and we will share proposed guidelines for implementing these strategies at the discovery and development stages, through scale up for production.

31. BASF's Socio-Eco-Efficiency Analysis: A Method for Evaluating the Economic, Environmental and Social Impacts of Products

Christopher A. Bradlee, BASF Corporation, Wyandotte, MI

In 2001 BASF SE began the process of integrating quantifiable social indicators into our existing eco-efficiency analysis methodology. The goal was to develop a quantitative life-cycle analysis methodology covering economic, environmental and social aspects of products and processes. Development was a part of a "Sustainable Chemistry of Aromatics" project and was a co-operative effort with Universität Karlsruhe (TH)—Institut für Geographie und Geoökologie and the Oeko-Institut eV.—Institute for Applied Ecology. In 2005 the SEEBalance® (Socio-Eco-Efficiency) methodology was introduced. Environmental and economic metrics are evaluated in accordance with BASF's Eco-Efficiency Analysis methodology. Social indicators were based on 1) Quality-of-life: Improvement of objective living conditions and improvement of subjective well-being; 2) Social Cohesion: Reduction of disparity and social exclusion and strengthening of social bonds and coherence; and 3) Sustainability: Intergenerational fairness and international responsibility. The metrics for the indicators were grouped into impact categories of employees, international community, future generation, consumer, and local and national community. To date BASF SE has initiated more than twelve SEEBalance® studies. Case study example is provided for garment manufacturing.

32. Benchmarking Sustainability

Darlene Schuster, AIChE Institute for Sustainability, Washington, DC, Subhas Sikdar, US EPA and Calvin B. Cobb, Institute for Sustainability, Cypress, TX

Various sustainability indices have appeared on the market, ranging from the AIChE Sustainability Index to financial sustainability indices. This presentation will discuss the roles of benchmarking sustainability performance and the utility of such benchmarks for the chemical industry as the approach greening along their supply chains

33. Environmental Decision Making and Metrics: Methodologies for Assessment and Sustainability

Sharon Austin, Environmental Protection Agency (U.S. EPA), Washington, DC

Environmental Footprint and Opportunities in Pharmaceutical Processes—Solvent Waste Streams as Secondary Product

A Green Engineering assessment of the pharmaceutical manufacturing process shows that solvents / waste solvents have the largest environmental footprint by far in natural resource usage, emissions of both toxic and GHG, and capital. The focus of this presentation that builds on this work will be on the opportunities presented in the recovery/reprocess/recycle and use of solvent waste streams. Models to calculate CO₂ and Energy requirements for post treatment (WWTP, incineration, energy recovery) and approaches in recovering, reprocessing of combined solvent waste streams based on basic physical chemical properties will be reviewed. Implications/opportunities with RCRA/OSW (recycling of RCRA waste), FDA/CDER (process optimizations affected by FDA registrations), and DOC/NIST (3rd party markets for recovered solvents) will also be reviewed.

35. Metal and Organic Solvent Free Green Oxidation of Alkyl Substituted Aromatics to Ketones and Carboxylic Acids with Aqueous *tert*-Butyl Hydroperoxide Under Microwave Irradiation

Albert W. M. Lee, Hao He and Bao-Jian Pei, Hong Kong Baptist University, Hong Kong, Hong Kong

Oxidation is the core technology to convert petrochemical based materials to commodity chemicals of higher oxidation state. However, oxidation reactions present some of the greatest challenges to the environment. Many of the industrial oxidation processes involved heavy metals or corrosive reagents, and are high in energy consumption.

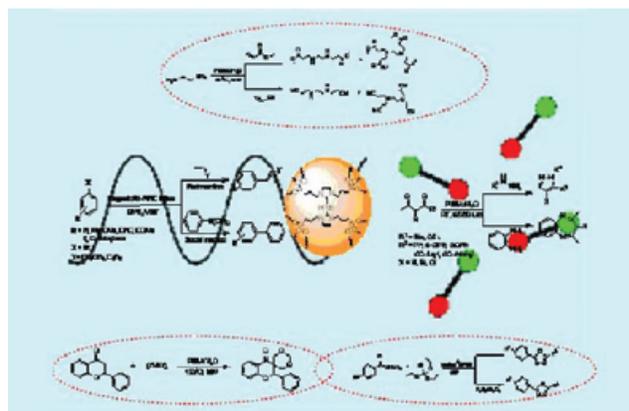
We have demonstrated that 70% aqueous TBHP (*tert*-butyl hydroperoxide) with microwave irradiation is a green oxidation protocol for alkyl substituted aromatics. Methyl aromatics (toluenes and xylenes) can be oxidized directly to the industrially important carboxylic and dicarboxylic acids. Addition of tiny amount of ionic liquid and simultaneous cooling improves the efficiency of these oxidations. For other alkyl substituted aromatics, ketones are obtained in good yields. The reaction medium is water. No organic solvents, metal based reagents or catalysts are needed.

The oxidation of xylene isomers to the corresponding phthalic acids open up a green alternative to the synthesis of these economically important fine chemicals. In the case of *p*-xylene, the oxidized terephthalic acids precipitated out from the reaction mixtures.

36. Greener and Rapid Synthesis of Bio-Active Heterocycles

Vivek Polshettiwar and Rajender, S. Varma, US EPA, Cincinnati, OH

A new kind of chemical revolution "GREEN CHEMISTRY" is brewing, 150 years after the first one transformed modern life with a host of conveniences. It protects the environment, not by cleaning up, but by inventing new chemistry and new chemical processes that do not pollute. The fundamental idea of green chemistry is that the manufacturer of a chemical is responsible for considering what will happen to the human life after the chemical is put in their society¹. Environmentally benign protocols have been developed for the synthesis of various bio-active heterocycles, which proceed under the influence of microwave irradiation and using eco-friendly conditions²⁻⁷.



References: (1) Curr. Opin. Drug Discov. Devel. 2007, 10, 723; Acc. Chem. Res. 2008, in press. (2) J. Org. Chem. 2007, 72, 7420. (3) Tetrahedron Lett. 2007, 48, 5649. (4) Tetrahedron Lett. 2007, 48, 7343. (5) Tetrahedron Lett. 2007, 48, 8735. (6) Tetrahedron Lett. 2008, 49, 397. (7) Tetrahedron Lett. 2008, 49, 879.

Abstracts, *Continued*

37. The “Greener” Leuckart Reaction

Mikhail M. Bobylev and Lioudmila I. Bobyleva, Minot State University, Minot, ND

The Leuckart reaction is a unique one step method of reductive amination. It is a remarkably simple process that includes only two components: the carbonyl compound and formamide. The reaction is completed simply by heating the components at 160°C to 185°C for 6 to 25 hours. The long processing time seems to be the only shortcoming of the reaction. However, it is associated with a number of serious practical problems. First, the prolonged exposure of the reaction mixture to high temperatures inevitably leads to significant thermal decomposition of the components, and, consequently, to lower yields of the products and large amounts of waste. Second, maintaining high temperatures for a long period of time means high consumption of energy and increasing production costs which make the Leuckart reaction unattractive to the chemical industry. In this work a fast non-microwave procedure for the Leuckart reaction was developed. The new procedure can be completed in minutes instead of hours. It minimizes the use of heat and practically eliminates any thermal decomposition of the reaction mixture. The specific examples of the reactions will be presented. The project is supported by NIH grant P20 RR016741 from the NCCR.

38. Fluorous Separation and Recycling Technologies for Green Organic Synthesis

Wei Zhang, University of Massachusetts-Boston, Boston, MA

This presentation highlights our four areas of research on the development of fluorous techniques for making organic synthesis a greener and more efficient process. 1) Fluorous molecules are lipo- and hydrophobic. This property has been utilized in the separation of fluorous molecules from non-fluorous organic molecules. Since recovered fluorous reagents and catalysts have minimal non-fluorous byproduct contamination, they generally can be reused for next round of reaction without significant effort on purification. 2) Microwave irradiation is an efficient and controllable energy source for organic synthesis. Many microwave reactions can be conducted under the solvent-free conditions. The combination of fluorous tagging strategy and microwave reactions can significantly reduce the reaction time and simplify the product purification process. This presentation will give several examples to demonstrate the good thermal stability and reactivity of fluorous molecules under microwave conditions. 3) Multicomponent reactions (MCRs) have a strong green chemistry aspect since the formation of a complex molecule can be accomplished in a one-pot reaction process that requires less energy and generates less waste. Fluorous tag-attached component can improve the purification efficiency of MCRs. They have been applied to Ugi/deBoc/cyclization reactions and 1,3-dipolar cycloaddition/Suzuki coupling reactions. 4) Catalysis is an important area of green chemistry research. The recent development of organocatalysis has provided a new approach to replace the use of toxic heavy metal catalysts. However, high catalyst loading and lack of general methods for catalyst recovery are two major issues associate with the organocatalysis. We have completed the synthesis of a fluorous version of imidazolidinone catalyst and compared it with the normal imidazolidinone in asymmetric Diels-Alder reactions. The fluorous catalyst has comparable reactivity and enantioselectivity, but the recovered fluorous catalyst has higher yield and purity. Extension of our preliminary results for making more fluorous recoverable organocatalysts will be discussed in the presentation.

39. Developing “Greener” Synthesis through Mechanochemistry

James Mack, Daniel C. Waddell, William C. Shearouse II, Maxwell Shumba and Philip A. Vogel, University of Cincinnati, Cincinnati, OH

Solvent has been considered a necessity in chemical reactions since the days of Aristotle. Even today it is believed that reactions conducted in solution are faster, more efficient and show greater reproducibility than those in the solid

state. Because of this, chemists have been trained to use solution phase chemistry in organic synthesis to such an extent that solid state chemistry is not considered. However, due to increasing interest in environmental protection and waste minimization, solid state chemistry has recently gained momentum. High speed ball milling (HSBM) has been developed as a solid state technique which may potentially rival solution phase chemistry. HSBM has been demonstrated to be equally fast, efficient and as reproducible as solution phase chemistry. HSBM can be conducted under a variety of conditions, mimicking solution phase chemistry for a variety of chemical reactions and procedures. Although methods have been developed to trap and dispose of solvent waste more efficiently, the ideal situation is to avoid generating the waste completely. In our research laboratory, we have developed safer, more environmentally benign method for reductions and oxidations using HSBM. We further look to develop a more fundamental understanding of chemical reactions via this unique reaction pathway.

40. Stabilized Alkali Metals for Safer, Sustainable Synthesis

Paul Vogt¹, Michael Lefenfeld¹ and Partha Nandi², (1)SiGNa Chemistry, Inc., Monmouth Junction, NJ, (2)Michigan State University, East Lansing, MI

With an affinity for donating electrons, alkali metals have enormous potential for speeding chemical reactions throughout science and industry—driving efficiencies in conventional industrial processes and enabling new pathways to clean energy and environmental remediation. However, that same high reactivity makes alkali metals unstable and dangerous to store and handle. Consequently, the metals have been largely dismissed by a generations' worth of applied chemists and avoided by industrial end users. SiGNa Chemistry, Inc. has discovered and developed a proprietary method for encapsulating alkali metals in nano-scale porous metal oxides. The resulting sand-like powders are stable at room temperature and take a significant amount of the danger and associated costs out of using reactive metals. More importantly, the SiGNa materials retain the chemical utility associated with the parent metal. This presentation will highlight SiGNa's green chemistry technology and how these novel materials drive fast and efficient reactions for a range of chemical processes, specifically Birch reductions. The Birch reduction is a one-electron reduction of aromatic rings with alkali metals (Li, Na, K) dissolved in liquid ammonia. Birch reductions are generally avoided for scale-up due to the complexities of the large-scale process and the hazards associated with the use of the metal and liquid ammonia on scale. A Birch reduction performed using SiGNa material removes the environmental and occupational hazards of alkali metals and does not require liquid ammonia or cryogenic temperatures. The SiGNa method improves yields, shortens reaction times, and simplifies workup procedures. Overall this presentation will demonstrate how SiGNa Chemistry has converted alkali metals from lab hazard to an essential component of industry's new green chemistry toolkit.

41. A Clean, Benign and Aqua Mediated Synthesis of Pharmacologically Active Spiro Heterocycles

Subhash C. Jain, Siva Panda, Pankaj Khanna and Sunita Bhagat, University of Delhi, Delhi, India

The chemistry of spiro heterocycles has been of considerable interest due to their pharmacodynamic nature and therapeutic importance. In continuation to our interest in the development of new bioactive heterocycles, we have recently found a clean, facile, ecofriendly and an economic route for the synthesis of some novel spiro heterocycles, viz. spiro[indol-pyrazolonyl-thiazolidines], spiro[indol-indozolyl-thiazolidines] and spiro[indol-benzoxazines] each containing different biodynamic moieties. These spiro heterocycles have been prepared via hitherto unknown Schiff's bases, which in turn were obtained by the reaction of indol-2, 3-diones with various aromatic and heterocyclic amines, under aqueous conditions, in 90–98% yield. Further, a series of various

biologically active symmetrical and unsymmetrical bis spiro indolyl compounds, containing alkyl and piperazinyl linkers, have also been synthesized using above developed methodology.

Some of these novel spiro heterocycles possessed anti-inflammatory, fungistatic, bacteriostatic and anti-convulsant activities; therefore all the above synthetic compounds have been screened for a broad spectrum of biological activities, in order to discover new pharmacophores for the future. Detailed synthetic methodology as well as the bio-activity data will be presented and discussed at the Conference.

42. Terephthalic Acid Synthesis at Higher Concentrations in High-Temperature Liquid Water

Mitsumasa Osada, Ichinoseki National College of Technology, Iwate, Japan and Phillip E. Savage, University of Michigan, Ann Arbor, MI

High-temperature liquid water (HTW) as a reaction medium is attractive for organic chemical synthesis because water is inexpensive, abundant, non-toxic, renewable, environmentally benign, and has desirable chemical properties. A particularly suitable large scale industrial reaction system for a HTW process is *p*-xylene oxidation to terephthalic acid. We have reported that high terephthalic acid yield and very low byproduct yields are available in HTW around 300°C. Though the technical feasibility of a HTW process for terephthalic acid synthesis has been demonstrated, one barrier that accompanies the HTW process at present is the low *p*-xylene concentrations (below 0.02 mol/L) that have been used experimentally. Low *p*-xylene concentrations mean low production of terephthalic acid per unit reactor volume. In this work, we conducted synthesis at higher concentrations of *p*-xylene, 0.2 mol/L, which is 10 times concentration of our previous work. To work at higher concentrations, though, involves running the reaction as a two-phase aqueous suspension since higher concentrations exceed the solubility of *p*-xylene in HTW.

We report new information concerning the effect of MnBr₂ catalyst concentration and oxygen feed method on the partial oxidation of *p*-xylene in HTW at 300°C. We used a 440 mL Hastelloy batch reactor for all experiments. Pure oxygen gas (O₂) was the oxidant and was fed into the batch reactor by syringe pump. Increasing the catalyst concentration slightly increased the reaction rate of terephthalic acid formation. The difference of oxygen feed method such as feed speed and amount significantly affected the *p*-xylene conversion and the terephthalic acid yield. The highest terephthalic yields (>90%) occurred at [*p*-xylene] = 0.2 mol/L, [O₂] = 1.8 mol/L, [Br] = 0.056 mol/L, and t = 130 min. These results indicate the feasibility of HTW for terephthalic acid synthesis at higher concentrations.

43. Piperylene Sulfone: A Fully Recyclable Smart Solvent to Couple Reactions and Separations

Veronica Llopis-Mestre, Daniele Vinci, Megan Donaldson, Pamela Pollet, Charles Liotta and Charles Eckert, Georgia Institute of Technology, Atlanta, GA

Solvents such as DMSO and DMF are excellent for organic reactions with inorganic salts because of their dipolar, aprotic and inexpensive character. But their high boiling points preclude benign separation and recycle. We report piperylene sulfone, a labile DMSO substitute, which undergoes a retro-chelotropic reaction into volatile species under modest conditions, and which can easily be collected and converted back into piperylene sulfone via a concerted reaction for re-use. This provides the opportunity for facilitating recovery and recycling of both catalyst as well as the solvent itself.

We have investigated the use of piperylene sulfone to couple separation and solvent and catalyst recycle with many reactions. As one example, we compare here its use for catalytic hydrogen transfer reactions with other organic solvents (DMSO, DMF, THF, acetone, toluene) and water. We reduced a series of aromatic ketones to their corresponding alcohols to demonstrate the stability to various functional groups. In all the cases, both a high conversion and enantiomeric excess were observed. The initial rate of the reduction reaction of acetophenone

in piperylene sulfone was higher than in the organic solvents studied but lower than in water. This solvent was successful as an immobilization medium for catalyst recycle as well.

44. Novel Biomimetic Catalysts for Green Polymerization in Water

Kei Saito, Monash University, Clayton, Australia

One of the critical factors in realizing a green chemical reaction process involves the choice of water, one of the greenest solvents, as the reaction solvent. Poly(2,6-dimethyl-1,4-phenylene oxide) (PPO), an important engineering plastic for electric household and automotive parts, has been produced by the oxidative polymerization of 2,6-dimethylphenol. This polymerization proceeds at room temperature, and it is an ideal atom economical reaction that does not require any leaving groups for producing the polymer. However, the polymerization is carried out using an organic solvent like toluene and benzene under oxygen. Therefore, both a solvent recovery process and an anti-explosive reactor are needed for industrial production. The use of water as the solvent for the oxidative polymerization to form PPO is the desired approach from a green chemical process. On the other hand, nature provides a molecular weight controlled and regioselective polymer under air at room temperature in water using an enzymatic polymerization. We believe using water is the key not only for the green chemical process but also to control the polymerization. From a green chemistry approach, we investigated a novel controlled polymerization to form PPO in water with a biomimetic catalyst.

45. Novel Biocomposites from the Fibers of Poultry Feather and Biopolymer

Masud Huda¹, Walter F. Schmidt² and Marc Tefreau¹, (1) Horticultural Research Institute, Washington, D.C., DC, (2) USDA/ARS/EMBU, Beltsville, MD

As an introduction for the sustainable/green engineering initiative, this study presents enabling processing technology needed to transform the fibers of poultry feather, a waste product left over after processing poultry in the food processing industry, as reinforcement filler material for manufacturing composite materials. We have successfully fabricated composite materials from biopolymer and fibers of poultry feather (FPF) with enhanced mechanical properties of the resulting compound. Innovative processing increased adhesion between the components. X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIR) were used to analyze the influence of treatments on the physical and thermal properties of fibers. Thermal behavior had also been studied by thermogravimetric analysis (TGA). Superior mechanical properties in composite materials were achieved. Scanning electron microscopy and Raman spectroscopy provided evidence of improved adhesion in the resulting composites at the microscopic and at the molecular level respectively.

46. Bio-Based Dielectric Materials for Printed Circuit Boards

Mingjiang Zhan and Richard P. Wool, University of Delaware, Newark, DE

Dielectric materials used for printed circuit applications consist of two components: the resin systems and the fiber reinforcement. The most successful and widely used resin systems are epoxy resin systems. However, the epoxy resin systems are petroleum-based which gives it some drawbacks, such as cost and sustainability issues. E-glass fibers have high dielectric constants which are not desirable for printed circuit boards. To solve these issues, a new soy oil resin was developed to replace the epoxy. Unsaturated soy oil was functionalized with different reactive groups to make it polymerizable. Then the functionalized oil was blended with comonomer and multifunctional agents to increase the crosslink density of the final thermoset. The resin system was designed to minimize the dielectric constants of the

Abstracts, Continued

thermoset in order to increase the operation speed of the printed circuits. Natural fibers such as keratin fibers from chicken feathers were treated and used as reinforcement. Carbonization process of fibers was optimized to give better mechanical and dielectric properties.

This project was supported by the National Research Initiative of the USDA Cooperative State Research, Education and Extension Service, grant number 2005-35504-16137.

47. Hydrogen Storage on Carbonized Chicken Feather Fibers

Erman Senoz and Richard P. Wool, University of Delaware, Newark, DE

Due to its environment-friendly features and high energy potential, hydrogen can be an ideal energy carrier for the future. However, there still are serious problems in the production and storage of hydrogen. The Department of Energy's (DOE) 2010 and 2015 hydrogen storage targets are quite challenging in terms of gravimetric capacity (6 wt% and 9 wt% respectively), volumetric capacity (45 and 81 grams H₂ per L), storage cost (\$4 and \$2 per kWh respectively) and practical usage i.e., safety, short refueling time and long cycle life. Chicken feather fibers (CFF), which are an agricultural waste, have great potential to become a main hydrogen storage material because of their hollow structure and low cost. When 92% keratin chicken feathers are carbonized by controlled pyrolysis, it is observed that the hollow structure of the keratin fibers does not change. Their surface area increases by the formation of fractals and micropores and their mean pore diameter decreases, thus enabling more hydrogen adsorption than raw (untreated) feather fibers. The main objectives of this study are investigating the details of the carbonization process of feather fibers, modifying and decorating their surface for higher hydrogen storage capacities. Hydrogen storage, pyrolysis, nitrogen adsorption, XPS and FTIR measurements will be presented.

This project was supported by the National Research Initiative of the USDA Cooperative State Research, Education and Extension Service, grant number 2005-35504-16137.

48. Renewable CARBON Nanospheres for Applications in Polymer Nanocomposites

Margaret Sobkowicz, John R. Dorgan, Keith W. Gnesin, Andrew M. Herring and J. Thomas McKinnon, Colorado School of Mines, Golden, CO

The dwindling petroleum supply along with climate change brought on by accelerating release of carbon into the atmosphere give rise to the demand for commodity plastic materials made from renewable resources. While several crop-based polymers are available on the market today, their full potential has yet to be realized due to thermomechanical property limitations. Nanocomposites offer the ability to control the polymer molecular interactions and thereby the bulk properties. Specifically, poly(L-lactic acid) (PLLA), produced from fermentation of corn sugars, is limited for packaging applications by its low heat distortion temperature and brittleness. PLLA is also slow to crystallize, which adds cost to processing operations.

Novel carbon nanospheres (CNS) derived from cellulose are a renewable nanomaterial that, when compounded with PLLA results in nanocomposites that are almost 100% renewable-based. In this study, various treatments of the CNS surface are compared in order to enhance the filler compatibility with the PLLA matrix. Chemically modified CNS show reversed solubility in non-polar solvents compared with the polar CNS as-received. The surface chemistries are characterized using thermogravimetric analysis, Fourier transform infrared spectroscopy, Raman spectroscopy and x-ray photoelectron spectroscopy. Performance of CNS as a nanofiller in PLLA is compared with common mineral fillers using a solution blending compounding technique. The resulting composites are characterized using thermal analysis and various mechanical testing techniques. Crystallization kinetics are explored in both the renewable PLLA and conventional polypropylene. The addition of CNS to the polymer

matrices leads to faster crystallization and shows promise for improved thermal and mechanical stability. The resulting materials can be considered a new class of ecologically responsible biopolymer nanocomposites.

49. Cellulosic Nanowhiskers: One-Step Functionalization and Use in Ecologically Benign Nanocomposites

Birgit Braun, PolyNew Inc, Golden, CO and John R. Dorgan, Colorado School of Mines, Golden, CO

Ecological concerns over the use of fossil resources and associated environmental degradation provide increasing motivation for developing renewable resources. The use of petroleum-based polymers for short product life packaging applications contributes to solid waste streams, leads to pollution of the oceans with plastic debris, and depletes increasingly precious natural resources. Plastics based on renewable resources (bioplastics) are emerging alternatives.

For many applications, the modification of mechanical and thermo-physical properties of bioplastics is desired. Cellulosic nanowhiskers (CNW) are attractive as filler material due to their exceptional mechanical properties as well as their renewable nature. However, dispersion in hydrophobic polymer matrices is difficult because of the hydrophilic nature of cellulose. Surface modifications usually involve the use of surfactants or multiple elaborate chemical steps. In this study, we present a one-step method for the isolation of CNW and their surface modification using renewable-based acetic acid. The slow hydrolysis kinetics of the organic acid can be partially overcome by a mixed acid system comprised of acetic and hydrochloric acid. In both cases, the presence of acetate groups is verified using spectroscopic techniques, and the surface degree of substitution of hydroxyl groups estimated using dimensional information obtained by multi-angle laser-light scattering. Solvent studies verify the increase in hydrophobicity. These novel functionalized CNW are subsequently incorporated into bioplastics to form nanocomposites.

50. DuPont™ Cerenol™—a New Family of Sustainable and Environmentally Friendly Materials

Hari B. Sunkara, E. I. du Pont de Nemours and Company, Wilmington, DE

DuPont's unique breadth of biology, chemistry and materials science has enabled the creation of DuPont™ Cerenol™, a proprietary new family of sustainable polymers that are built on principles of green chemistry. This presentation emphasizes the significant impact of this innovative technology platform on society, environment, and human health, and its broad applicability in industry. Cerenol™ can serve as an alternative to synthetic polyalkylene glycols which rely on high cost crude oil and natural gas feedstocks. Cerenol™ process uses a renewably sourced and inherently safer raw material, and is less material intensive and more energy efficient. The result is a reduction of green house gas emissions over traditional processes. We have demonstrated and patented the broad applicability of the Cerenol™ polymers in coatings, inks, functional fluids, lubricants, personal care, specialty elastomers, polymer blends, and fibers. This novel technology provides an excellent platform for future renewably sourced products and elastomers and thus contributes to reduce the chemical industry's dependence on petroleum.

51. Elimination of Hexavalent Chromium Used in Hydraulic and Pneumatic Tubing

Robert R. Rick, Commercial Fluid Power, La Porte, IN

Commercial Fluid Power in conjunction with MACSTEEL NitroSteel Division has developed a tubing product that replaces Chrome Plated Interior Diameter (CPID) tubing and Chrome Plated Outside Diameter (CPOD) tubing used in the manufacturing of hydraulic and pneumatic cylinders. Precision machined tubing products are Ferritic Nitro-Carburized (FNC) and oxidized giving the surface a hard chrome like wear surface, good lubricity, a low co-efficient of friction

and better corrosion resistance than standard CPID and CPOD products. The primary focus on this technology development has been to eliminate hexavalent chrome, a toxic, carcinogenic substance that is created in the production and disposal of CPID and CPOD tubing. The Ferritic Nitro-Carburizing and Oxidizing of these precision machined parts waste product is water. This Nitriding and Oxidizing process's impact on the environment is very minimal compared to the waste products generated by industrial hard chrome plating with the current technology that exists today. This product, as developed, is a direct replacement material for Chrome Plated OD and ID tubes. There is no hazardous by products produced in the manufacturing of Nitro-tuff tubes or in the disposal of this product after it has served its useful life. Nitro-tuff Pneumatic Cylinder Base: Material St52.3 SRA DOM Produced to ASTM A513 Type 5 Nitro-tuff Hydraulic Cylinder Base: Material 4130 Q&T 28/32 HRC with a 100% Martensitic Grain structure Surface Thickness: 0.001" minimum thickness per side. Diffusion Zone: Hardened diffusion zone, beneath the wear layer, has a hardness gradient from low 50's Rc to = 40 Rc at 0.015" depth. Surface Finish: 16 Ra Maximum Corrosion Resistance: 150 Hours in a Neutral Salt Spray Bath with a Rating 10. Tested and rated per ASTM B117 and B537. In summary Nitro-tuff tubes are an eco friendly, cost effective replacement for CPOD and CPID tubing.

52. Improved Control of Organic Sulfur

Stephen A. Bedell, The Dow Chemical Company, Lake Jackson, TX

Mercaptans are often found in natural gas and refinery waste streams and have traditionally been among the most difficult of sulfur compounds to deal with. Though scrubbing with amine solvents is an excellent way to remove hydrogen sulfide, such technologies are limited in the amount of mercaptan removal that can be accomplished. Failure to adequately remove organic sulfur compounds in the amine scrubber results in one of two environmental problems; use of caustic scrubbers for mercaptan removal results in hard to treat mercaptide or disulfide waste products, or the sulfur ends up at higher levels in various hydrocarbon fractions which are used as fuels. A novel mercaptan removal technology will be presented which allow the existing amine scrubbers to remove substantially higher levels of mercaptans. New views of mercaptan/ amine chemistry will be presented along with commercial testing results.

53. A Novel Solid Catalyst Process for Biodiesel Production

Dheeban Kannan and Jack V. Matson, The Pennsylvania State University, University Park, PA

Biodiesel, a renewable fuel, is an important alternative energy option in terms of energy, environment, and economy. Biodiesel is produced from vegetable oil (algae-oil, animal tallow and used oil can also be used) and alcohol by transesterification reaction with glycerol as by-product. Current methods use soluble catalysts (60°C, ~100 min) that pose separation and product contamination issues. Our idea was to use solid catalysts to produce biodiesel employing ethanol as a critical fluid medium as well as a reactant. Critical region of the alcohol is desired for the mixing of alcohol and oil phases, which are otherwise immiscible, to minimize mass transfer limitations. The aim was to develop a continuous process (packed bed) for commercial biodiesel production. Metal oxides, manganese oxide, titanium oxide, calcium titanate, calcium aluminum oxide and copper oxide, were identified as effective solid catalysts from batch tests. Critical reaction regime (260°C, 1000 psi) gives conversions ~95% in 5~20 min. The process can handle feedstock with high free acid content (to exploit cheap feedstock) unlike the conventional process that requires an additional acid-catalyzed step preceding the main base-catalyzed step. Catalysts have been tested successfully against performance deterioration over time. The process eliminates additional processing units associated with the conventional process, such as, separate catalyst-alcohol mixing unit before reactor, catalyst neutralization unit, water-washing steps to remove soap and catalyst, and, contaminated glycerol refining unit. The process

will not have waste water disposal problems unlike the conventional process. The process can be termed as totally green. Biodiesel potential and pending studies would be discussed.

54. Developments in REACTOR Engineering: MODELING of Gas—Phase Catalytic Channel Reactors

Alex Omo Ibhadon¹, Polycarpus Falaras² and Dimitris Tsoukleris², (1)University of Hull, Hull, United Kingdom, (2)Institute of Physical Chemistry, Athens, Greece

Experimentally validated designs of two catalytic reactors, a Channel Gas-Phase reactor with photoelectrochemical enhancement (PE) and a Packed Bed Reactor is reported. Modeling studies involving kinetic and mass transfer parameters, surface reactions, the effect of light absorption on the reactions and reactor geometry, indicate that the reactors can be used for gas-phase heterogeneous oxidation reactions.

The Channel reactor is characterized in terms of the permeability and gas to solid mass transport. In the latter case, this is achieved by performing limiting current techniques using a liquid with the same Reynolds numbers as expected for the gas phase system. A mathematical model was developed to bring together the transport and mass transport behaviour of the reactor with the kinetics of the photocatalytic reactions as determined experimentally and the fluid flow behaviour enabling the simulation of the effect of temperature, concentration of contaminants, pressure, wavelength and light intensity on reactant conversion. The fluid flow distribution is modeled two dimensionally to allow the determination of fluid residence time distributions through the catalyst microstructure and any potential inactive zones.

The Channel reactor is optimized by varying the residence time, channel dimensions and the characteristics of the catalyst used including the thickness. A novel feature of the Channel reactor is the introduction of photoelectrochemical (PE) enhancement to suppress electron-hole recombination. This first attempt to carry out gas phase photo-electrochemical oxidation required the optimization of the electrode structure, thickness and ionomer content, achieved both by modeling the current distribution and experimentation. Results indicate that varying the structural parameters, measuring photocurrent and electrode response in a solid-state cell enabled the simulation of the actual PEC reactor.

55. Extension of the Environmentally Benign Catecholate Method to the Synthesis of Barium-Based Perovskites and Environmentally Benign Synthesis of Doped Barium Titanate

Anne E. Marteel-Parrish, Danielle Harlan, Jonathan Martin, Samantha DeCarlo and Heather Sheridan, Washington College, Chestertown, MD

Barium titanate (BaTiO₃), barium zirconate (BaZrO₃), barium hafnate (BaHfO₃), and barium stannate (BaSnO₃), are all essential components of the electroceramic industry. Barium titanate is the most well known member of the perovskite family primarily used for multi-layered ceramic capacitors in computers, aerospace, and communication technologies. Barium zirconate is one of the most inert, stable, and corrosion-resistant perovskite employed in superconducting applications. Hafnium-based oxides are currently leading candidates to replace silicon oxide as a gate insulator in field effect transistors. Barium stannate is mostly used as a sensor material. The first goal of this research was to apply a more efficient and environmentally benign synthesis design to the production of barium-based perovskites. The catecholate method, which was originally applied to the synthesis of barium titanate, was used as the approach for the synthesis of barium zirconate, hafnate, and stannate. This method consumes naturally occurring and less toxic precursors, smaller quantities of solvents, and results in the absence of by-products while achieving stoichiometric control over the barium-to-X (X= Ti, Zr, Hf, Sn) molar ratio. The second goal of this research was to develop a greener alternative

Abstracts, *Continued*

to the doping of barium titanate. For barium titanate to be used as a capacitor, a high dielectric constant is needed at room temperature which is achieved through doping. The barium source was barium titanyl catecholate trihydrate ($\text{Ba}[\text{Ti}(\text{cat})_2] \cdot 3\text{H}_2\text{O}$) and the doping sources were strontium oxalate (SrC_2O_4) and strontium carbonate (SrCO_3). The two doping strategies were a microwave- and a centrifuge-assisted method which used water as a solvent. These methods allowed thermodynamic control over barium-to-strontium molar stoichiometric ratios. X-ray powder diffraction, infrared spectroscopy, and inductively coupled plasma were used to analyze all final powders. The doping strategies, characterization data, and outcomes are detailed in this presentation.

56. Biomass-to-Liquids (BTL): The Green Fuel of the Future?

Jeff McDaniel and Dave Kilanowski, Velocys, Inc., Plain City, OH

Sustained high oil prices, concern about global climate change, and the drive for energy security are intensifying the search for alternative fuels. First generation biofuels, including corn ethanol and biodiesel, are prevalent today; however, these are seen as only an interim solution due to their use of food crops for raw material. Next generation biofuels, ones that use non-food biomass, are a more sustainable choice. These include biomass-to-liquids (BTL) via gasification and Fischer-Tropsch synthesis. This process produces a high quality, energy dense fuel from a wide variety of resources, including waste wood, energy crops and municipal solid waste.

The synthetic diesel produced from a Fischer-Tropsch based facility is a superior fuel that can be used as a one-to-one replacement for petroleum-derived diesel or jet fuel. In fact, the very high Cetane Number and low sulfur content of synthetic fuels actually improve engine performance for many applications.

The concept of producing synthetic fuels in compact units hinges on the ability to cost effectively scale-down reaction hardware while maintaining sufficient capacity. By greatly reducing the size and cost of chemical processing hardware, systems based on microchannel process technology hold the potential to do just this. Reactors using this technology are characterized by parallel arrays of microchannels, with typical dimensions in the 0.01 to 0.2 inch range. Processes are intensified by reducing heat and mass transfer distances, thus decreasing resistance between process fluids and channel walls. Overall system volumes are typically reduced 10- to 100-fold or more compared with conventional hardware.

This presentation will discuss a rapidly deployable microchannel-based synthetic fuels process, under development at Velocys Incorporated of Plain City, Ohio. The presentation will cover technical development, environmental impacts and the use of synthetic fuels in automobiles and commercial vehicles.

58. Greening Analytical Chemistry Education: Expanding the Green Revolution

Liz Gron, Hendrix College, Conway, AR

Green chemistry principles have the potential to reshape how we do business. These transformational principles remove the artificial constructs that place economics at odds with environmental stewardship allowing for increased sustainability of health and wealth. Although the importance of green chemistry is clear, the development of green chemistry curriculum has been spotty. In particular, analytical chemists are responsible for developing the methods to acquire the essential data necessary to evaluate system health; but analytical chemists are relative newcomers to the field of green chemistry. This paper describes the novel innovations in analytical chemistry that are making it possible to acquire data using increasingly greener methods, identifies existing green analytical methods, as well as presents new educational materials to teach the green mind-set to our analytical students. This paper will give an overview of green analytical methods, primarily innovations in sample pretreatment, while describing the developments and possibilities for green undergraduate analytical materials in introductory laboratories.

59. Development of a Green Inorganic Chemistry Laboratory: Principles, Practices and Procedures

Indu Tucker Sidhwani, Gargi College, University of Delhi, New Delhi, India and R.K. Sharma, University of Delhi, Delhi, India

Gargi College is one of the two colleges in Delhi, out of 65, selected by the University Grants Commission of India as a college with potential for excellence. As Green Chemistry is becoming an important issue in industry, research institutions and the society, students at all levels can benefit from introduction to Green Chemistry. So it was decided that approval be taken from UGC under the 'cpe' scheme for greening of some of the existing experiments and introducing some new green experiments. This has been done with the aim of introducing Green Chemistry principles and chemical concepts to undergraduate students in an integrated manner. Some of the experiments like 'Greener Alternatives to Qualitative Analysis of Cations, 'Preparation of Blue and Green Fluorescent Isomers of tris(8-hydroxyquinolino)Al(III)' and many more will be discussed. In each experiment, it is shown as to how green methods are following Green Chemistry principles in addition to the chemical concepts. Some of these experiments developed by us are part of an add-on course on Green Chemistry of other colleges, like Miranda House of the University of Delhi. Some of these experiments have also been incorporated in a monograph of Green Chemistry Experiments by Sharma, Sidhwani and Chaudhuri, which was distributed as reading material in the 3rd Indo-US S and T Workshop of Green Chemistry in Delhi, India (7-9 January, 2008). We are also in a process of designing more green inorganic chemistry experiments for the curriculum.

60. An Undergraduate Research Experience in Green Chemistry: Exploring An Immobilization Strategy for a Heterogeneous Catalyst

Corey A. Mocka and Denyce K. Wicht, Suffolk University, Boston, MA

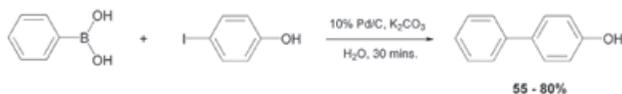
In the College of Arts and Sciences at Suffolk University, all undergraduate students pursuing a degree in chemistry or biochemistry must complete a research course in order to fulfill the degree requirements. The senior thesis is a yearlong endeavor in which a student works closely with one faculty member on an in-depth review paper, a mock grant proposal, or a laboratory research project. In this talk, the details of an undergraduate green chemistry laboratory-based research project will be discussed. Specifically, an experiment focusing on novel catalyst synthesis via siloxane condensation was explored. This investigation into the synthesis of cross-linked siloxane in which a model catalyst, trimethyl-[3(triethoxysilyl)propyl] ammonium chloride, was covalently bonded to the material will be presented. Non-toxic anionic dyes were used to probe electrostatic interactions in the siloxane between the dyes and the quaternary ammonium salt. The research utilized basic organic techniques resulting in the synthesis of thermoset siloxane polymers. Overall, this project provided valuable multi-disciplinary research training and allowed for the development of expertise in the laboratory application of green chemistry principles.

61. "Greening up" Organic Reactivity in the Undergraduate Laboratory: Aqueous Horner-Wadsworth-Emmons, Heck and Suzuki Reactions

Andrew P. Dicks, University of Toronto, Toronto, ON, Canada

There is currently significant interest in undertaking organic reactions under purely aqueous conditions, both in an academic and industrial climate. Water is the cheapest solvent on Earth; it has no flammability issues; it alleviates pollution problems associated with organic media and often engenders improved synthetic efficiency. The incorporation of three microscale synthetic experiments into the third-year organic chemistry undergraduate curriculum will be discussed. Each experiment involves usage of water as the solvent for a carbon-carbon bond forming process. Adoption of this approach facilitates

synthesis of cinnamate ester sunscreen analogs via a Horner-Wadsworth-Emmons reaction and preparation of non-steroidal anti-inflammatory drug analogs via a Suzuki reaction (below), thus showcasing the “real-world relevance” aspect of organic chemistry to students.



62. Green Chemistry Networking in India

R. K. Sharma, University of Delhi, Delhi, India

Green Chemistry Network Centre (GCNC) established in Delhi University under the recommendation of a panel of world leaders headed by Professor Paul T. Anastas (known as father of Green Chemistry) is working for the Green Chemistry education and outreach activities in India by:

- Building a Network for exchange of expertise, discussion and knowledge between industrialists and academicians.
- Preparing and disseminating the teaching materials on Green Chemistry for school, college and university levels, with the simultaneous design of laboratory experiments for these levels as well.
- Designing trainings
- Translating existing Green Chemistry materials for broader distribution through the network all over India.

Recently to strengthen the Green Chemistry Networking in India, GCNC organized INDO-US S&T Forum Workshop on Green Chemistry on 7–9 January at Delhi. A stepping stone in the endeavors of GCNC was the release of a monograph on Green Chemistry Experiments in this workshop. Green Chemistry Task Force created by Department of Science & Technology, Government of India for the furtherance of Green Chemistry Education & Research in India recently invited Coordinator of GCNC for preparing a Green Chemistry Experiment Manual. This manual will be recommended for all the University and Colleges of India for its inclusion in the existing curriculum. Green Chemistry Network Centre (GCNC) has been instrumental in getting Green Chemistry courses introduced at the Bachelor's level in University of Delhi. More interesting educational initiatives taken are in the form of value based short-term courses on Green Chemistry that incorporate laboratory experiments, case studies etc. contribute in the furtherance of the much needed science. This presentation will describe the overall educational and outreach activities of the centre.

63. Infusing Sustainability and Additional Green Chemistry into Chemistry in Context

Michael C. Cann, University of Scranton, Scranton, PA

In 1994 the first edition of Chemistry in Context (a project of the ACS) was published. This work, for non-science majors, was a groundbreaking book in that it taught chemistry in the context of major social, political, economic and ethical issues on a “need to know” basis. Another groundbreaking event for this book occurred in the 3rd edition (2000) with the infusion of modest amounts of green chemistry. For the 7th edition, the editor-in-chief (Catherine Middlecamp) has set a goal of having sustainability and green chemistry as major theme throughout the text. This goal is in harmony with the ACS mission statement¹ “To advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people” and a 2005 ACS report² that concluded “By 2015, the chemistry enterprise will be judged under a new paradigm of sustainability. Sustainable operations will become both economically and ethically essential.” This presentation will highlight some of the issues and examples of sustainability and green chemistry that relate to the content of this text.

References: (1) http://portal.acs.org/portal/acs/corg/content?_nfpb=true&_pageLabel=PP_ARTICLE_MAIN&node_id=1390&content_id=WPCP_007471&use_sec=true&sec_url_var=region1 (2) <http://chemistry.org/chemistryenterprise2015.html>

64. A Study of Ganoderma Amboinense Lanostanoid Triterpene

Lou-sing Kan and Hung-Chieh Lu, Academia Sinica, Taipei, Japan

Ganoderma plant has been used extensively in the Chinese herbal therapies for centuries due to its bioactivities derived from the lanostanoid triterpenes ingredients. This paper introduces the superior supercritical fluid extractions (SFE) for these triterpenes for saving the consumption of time and organic solvents. The thrift of latter item in purification and separation will benefit the environment. The yield of lanosta-7,9(11),24-trien-3-one,26,27-dihydroxy-(9C) (GA), for an example, by SCF is 70% higher than that obtained by traditional organic solvent extractions. In consequence, a sufficient sample can be obtained for ¹³C and ¹H NMR studies. The chemical shifts of triterpenes were unambiguously assigned by varies 1D and 2D NMR spectroscopy. Both the fused ring structure and the side chain structure were elucidated from the ¹³C-¹H correlation NMR spectra. The absolute configuration about the chiral carbon was determined by NOE NMR spectra. Thus, the structure and the absolute configurations of the chiral carbons of GA have been determined. The structural information of GA will facilitate the further development of drug design. (Acknowledgement to the High-Field Biomacromolecular NMR Core Facility supported by the National Research Program for Genomic Medicine and Academia Sinica, Taiwan)

65. Commercial Viable Resolution of (S)-Ibuprofen

David Chavez and James Salvador, University of Texas at El Paso, El Paso, TX

Enzymatic esterification of racemic ibuprofen catalyzed by *Candida rugosa* lipase in cyclohexane at 40°C was developed with high selectivity for (S)-ibuprofen over the (R)-ibuprofen enantiomer. The length of the alcohol used changed the velocity of the esterification from 48 hours for decal-1-ol to 96 hours for butan-1-ol. Esterification with decan-1-ol was more enantioselective than that of butan-1-ol as measured by their respective enantiomeric ratios, E, 130 and 46.

Bulb to bulb distillation of (R)-ibuprofen and decan-1-ol from the (S)-decyl ibuprofen ester, besides not requiring solvents, was run at a larger scale than chromatography. Bulb to bulb separation of ibuprofen from the butyl ibuprofen was not effective because of the close boiling points of carboxylic acid and ester. As expected total hydrolysis of (S)-ibuprofen esters in the native solvent of lipase, water, was possible although the reaction of the decyl ibuprofen ester was half as slow (48 hours) as the reaction of the butyl ibuprofen ester probably because of the lower solubility of the decyl ester in water. Nevertheless the combined time of esterification and hydrolysis of decyl and butyl ibuprofen esters was comparable.

Chiral HPLC analysis demonstrates that pure (S)-ibuprofen was isolated, without racemization, by enzymatic esterification of racemic ibuprofen with decan-1-ol, effective and efficient bulb to bulb distillation and separation of products, and environmentally benign hydrolysis of the (S)-decyl ibuprofen ester with the same *Candida rugosa* lipase

66. Soy-Based Polyols for Polyurethane Applications

Zuleica Lozada and Galen J. Suppes, University of Missouri-Columbia, Columbia, MO

The developments of polyols bio-based are growing for decades and its going to replace petroleum-based polyols. Soy-based polyols are potentially low-cost materials and reduced impact on the environment. In addition, the introduction of natural oils into the polyurethane products can provide an opportunity for suppliers and customers to reduce their dependence on crude oil from

Abstracts, *Continued*

petroleum. The present work proposes a few new soy-based polyols which are produced by oligomerization of triglycerides (or derivatives of triglycerides) and have good reactivity with isocyanate in elastomers, rigid and flexible polyurethane foam production. New soy-based polyols have been synthesized based on epoxidation and alcohol moieties attached to bodied soybean oil. Rigid, flexible, and elastomer polyols have been synthesized and reacted to from urethanes with a range of properties. The used of the bodied fatty acid backbone was effective to increase the functionality and/or hydroxyl equivalent molecular weight. Some of the soy-based polyol proposed have disadvantages associated with increase number and/or complexity of process steps, but at least the final product has a good quality. The proposed methods increase the molecular weight of the triglyceride to average values over 1500.

67. Use of Highly Nanoporous Carbon in Batteries and Supercapacitors

Sean P. Crockett, Ali Tekeei, Michael Gordon, Bryan D. Sawyer, Matt Wopata and Galen J. Suppes, University of Missouri-Columbia, Columbia, MO

A nanoporous carbon with tunable porosities and surface areas in excess of 3,000 m²/g has been developed and is being evaluated in a number of supercapacitor and battery architectures. This presentation is on an approach that presses the carbon into a monolith structure that can be machined to electrodes.

Electrodes have been fabricated for lead-acid batteries toward the goal of improving deep cycle endurance and increasing energy density. The carbon provides a robust grid with reduced adverse effects from the expansion/contraction cycles that greatly reduce cycle life of traditional lead-acid batteries. Data will be presented on fabrication and performance.

68. Photocatalytic Degradation of Omethoate Using Ti-Containing Zeolite

Dishun Zhao and Jialei Wang, Hebei University of Science and Technology, Shijiazhuang, China

Photocatalytic oxidation of Omethoate with hydrogen peroxide using Ti-containing zeolite (TS-1) as photocatalyst at ultraviolet lamp irradiation had been studied. The effect of the photocatalyst amount, pH, hydrogen peroxide concentration and the radiation time on the degradation ratio of Omethoate were investigated in detail. Kinetics parameters of the photocatalytic oxidation of Omethoate were measured and calculated. The result shows the kinetics of photocatalytic oxidation of Omethoate is first-order. The activity of photocatalyst was not decreased obviously after reused for five times. Using this photocatalytic oxidation system can effectively reduce the Omethoate content in water. Under experimental conditions, the removal ratio of Omethoate is up to 93%.

69. Surface Modified Silica Supported Zinc Salicyldimine Complex for Use as Catalyst in Transesterification: A Green Chemistry Approach

Anju Srivastava, R.K. Sharma and Deepti Rawat, University of Delhi, Delhi, India

Transesterification is an important organic reaction that can be used to synthesize various intermediates in the synthesis of complex natural products, pheromones, polymers and paint additives. Its value has been considerably enhanced by its use as a key step in the manufacture of biodiesel, one of the more environmentally friendly and sustainable fuels we have available today. Transesterification reactions mostly proceed using expensive homogeneous organometallic catalysts, strong acids and soluble bases, none of which is ideal from a green chemistry perspective. They are incompatible to the modern synthetic industrial chemistry that desires to be highly efficient, selective, ecofriendly and preferably catalytic.

One of the most important current topics in catalysis is the development of efficient and environmentally friendly polymer supported catalyst for carrying out various organic reactions for industrial purposes. In spite of the high activity, the application of homogeneous catalysts has declined in past years due to several problems, particularly the decomposition or degradation of the catalyst following a variety of pathways such as auto-oxidation, ligand decomposition and separation. Therefore, one of the challenges in green chemistry is to develop highly selective heterogenized homogeneous catalysts. Immobilization of molecular homogeneous catalysts is a promising approach that offers a dual advantage of selectivity and activity of the homogeneous catalyst as well as the ease of separation and re-usability of the heterogeneous catalyst.

In the present work, we have carried out the immobilization of zinc salicyldimine complex on silica and evaluated its catalytic activity for transesterification.

This new approach to immobilization of complexes exhibits promise in tailoring synthesis of highly active, stable and reusable catalysts for specialized reactions.

70. Chemically Modified Fatty Acid Methyl Ester and Its Use in Vinyl Ester Resins

Alejandrina Campanella, Gregory Stirparo, Michael Zeberkiewicz and Richard P. Wool, University of Delaware, Newark, DE

Vinyl ester (VE) resins that are employed in many commercial applications need diluents to allow the resins to be molded using liquid molding techniques. These diluents are typically volatile organic compounds that should be avoided to reduce health and environmental risks. Therefore, chemically modified fatty acid methyl ester (CMFAME) from soybean and linseed oil were synthesized and employed as a diluent for VE resins. The effect of the weight ratio of CMFAME to VE on the resin and polymer were analyzed by studying the rheometric and mechanical properties, respectively. The viscosity of these resins and the mechanical properties of the bio-based polymers were analyzed. The viscosity of VE/CMFAME resins and glass transition decreased as the content of CMFAME increased. These resins have properties that are comparable to commercial resins. Also, a chemical modified lignin (butyrate kraft lignin) was added to these resins (VE/CMFAME) and the mechanical properties of the polymer were improved.

71. Green Engineering Design for the Recovery of Solvents in API Manufacturing

Anthony J. Furiato, Kyle E. Lynch, Timothy M. Moroz, Mariano J. Savelski and C. Stewart Slater, Rowan University, Glassboro, NJ

The pharmaceutical industry is constantly exploring methods for process optimization and improvement. Reduction of solvent use and recovery of waste solvents are issues of importance in most API (Active Pharmaceutical Ingredient) manufacturing processes. Process waste streams are often characterized by high volumes of organic solvents that sometimes are difficult to recover and reuse due to azeotropes, resulting in high cost of waste disposal and a large life cycle environmental footprint. Solvent recovery and reuse operations must meet stringent pharmaceutical industry requirements for solvent purity. Rowan University and Pfizer have collaborated to explore green engineering alternatives for waste minimizing solvent recovery processes for the Celecoxib process. A case study has been performed that explores pollution prevention and remission opportunities for the current process. Two viable techniques, pervaporation-distillation hybrids and extractive distillation, have been identified to treat the process waste. The case study describes equipment and processing issues, financial costs and benefits; and environmental impacts through life cycle assessment techniques.

72. Bodied Soybean Oil Hydroxylation Via Transesterification

Arnold Lubguban, Yuan-Chan Tu, Zuleica Lozada, Fu-hung Hsieh and Galen J. Suppes, University of Missouri-Columbia, Columbia, MO

A high-molecular weight hydroxylated acylglycerol-based molecule was initially synthesized by thermally polymerizing soybean oil in a Diels-Alder formation, a mechanism whereby crosslinking of acylglycerols generally occurs at the 2-position of the fatty acid moieties. Hydroxylation was achieved by direct heat treatment of the polymerized or bodied soybean oil and pure glycerol. This thermal route involves transesterification in a closed reaction of the macromolecule with glycerol at temperatures greater than 200°C. Tunability in the functionality of the molecule through hydroxylation was achieved. In addition, the method effects a significant increase in molecular weight of the macromolecule with respect to processing time. Control of the parameters mentioned translate to a synthesized product with the desired functionality and molecular weight for vast practical chemical applications that include polyols in polyurethane production. Rigid foaming results of the processed soy-based polyol showed excellent physicochemical properties suggesting comparability with a petroleum-based polyether polyol.

73. Mechanical Properties of Water-Blown Flexible Polyurethane Foams Containing Epoxidized Soybean Oil

Yuan-CHAN TU, Hongyu Fan, Galen Suppes and Fu-hung Hsieh, University of Missouri-Columbia, Columbia, MO

Water-blown flexible polyurethane foams were made by replacing 0 to 50% of Voranol® 4701 with epoxidized soybean oil (ESBO) in the B-side of foam formulation and PAPI® 27. The density, 50% compression force deflection (CFD), 50% constant deflection compression (CDC), tear and resilience of foams were determined. Molded plastic strips were also made by replacing 0–50% Voranol® 4701 with epoxidized soybean oil and PAPI® 27. Dynamic mechanical spectrometer (DMS) and differential scanning calorimeter (DSC) were used to determine the hard and soft segments and thermal properties of these plastic strips. The density of water-blown polyurethane foams decreased first when introducing ESBO into the foaming system and then increased. The 50% CFD trend was similar to that of density. The 50% CDC of foams increased and resilience decreased when introducing ESBO into the foaming system. The DMS results show that the peak of tan delta decreased with increasing epoxidized soybean oil content indicating that the hard segment increased with increasing epoxidized soybean oil content. The DSC results reveal that the ΔC_p decreased with increasing epoxidized soybean oil content indicating that the soft segment decreased with increasing epoxidized soybean oil content.

74. Towards Characterizing the Active Coagulation Agent in *Opuntia* Spp

Sarah M. Miller and Julie B. Zimmerman, Yale University, New Haven, CT

Opuntia spp., a type of cactus, grows in many water-scarce regions. This plant has myriad uses, ranging from cuisine in some cultures to cattle feedstock to coagulating agent for water clarification. This project investigates *Opuntia* spp. for application as a point-of-use water treatment technology. Unlike some coagulants used in centralized water treatment, *Opuntia* spp. is of natural origin, renewable, and not associated with any ecotoxicological or human health concerns. *Opuntia* spp. is able to remove 98% of turbidity from synthetic turbid waters, and it was recently hypothesized that *Opuntia* spp. operates through a bridging coagulation mechanism. The active agents responsible for coagulation have not yet been isolated. This research establishes which parts of the *Opuntia* spp. cladode demonstrate coagulation activity. In addition, results on the charge, size, and molecular form of the active agent are presented.

75. Glycerin Carbonate—a Unique and Versatile Chemical

Mark L. Posey, Haibo Zhao and Vincent Zhang, Huntsman Corporation, The Woodlands, TX

Glycerin carbonate (GC) is unique among the family of cyclic carbonates in that it has two reactive sites. The hydroxyl group also gives the molecule unique solvency and reactive possibilities. The various chemical routes to the formation of glycerin carbonate will be discussed. Although many routes have been studied, one route seems to elevate itself as the most commercially and economically attractive choice. As GC is made from glycerin, which in turn comes from transesterification of vegetable oils, it has a high renewably sourced content, which is a positive in many markets today.

Many example commercial uses for glycerin carbonate will be presented. Examples of uses are as a solvent in personal care, as a CO₂ absorption solvent, polycarbonate raw material and as a reactive solvent in polyurethane coatings, among many other uses. The unique physical properties of glycerin carbonate will be discussed. GC has a very low vapor pressure making it an ideal low odor solvent. Its toxicity profile is also favorable given that it decomposes back to benign glycerin in the environment.

Glycerin carbonate is commercially available today and is TSCA and EINECS registered. However, GC has not been able to find large scale use in the past due to the high cost of manufacture. Huntsman is developing a proprietary process that will break through the cost barriers that should allow more widespread use in a variety of applications.

76. Gold Compounds with Tripodal Bis(imidazole) Thioether Ligands as Oxidation Catalysts

Reema Anis, Fangwei Liu, Eunmi Hwang and Maria Contel, Brooklyn College and the Graduate Center, The City University of New York, Brooklyn, NY

The synthesis of less toxic oxidation catalysts is of much interest in green chemistry. Due to a significant untapped potential gold homogeneous catalysis is only now recognized a scientific hotspot¹ with an increasing number of publications appearing on a weekly basis. The significance of Au(I) and Au(III) complexes as homogeneous catalysts for several reactions has been only recently addressed.² There is still a need, however, to fully understand reaction mechanisms in order to rationally design more efficient and selective catalysts. One of the areas in homogeneous gold catalysis that has received much less attention has been selective oxidation, particularly using molecular oxygen. Gold(I) complexes have been effective in the oxidation of alcohols (with molecular oxygen)³ and the oxidation of alkenes.⁴ The nature and oxidation state of the active catalytic species is still not known. We are interested in the synthesis of gold compounds in different oxidation states (I and III) with the same set of ligands and their use in different catalytic processes.

We present here the preparation of new gold compounds with tripodal bis(imidazole) thioether ligands that have different heteroatoms (nitrogen and sulfur) than can act as donor atoms to the gold centers. This ligand system can thus stabilize gold(III) and gold(I) complexes and may allow the identification of some reaction intermediates in oxidation reactions. Results for the catalytic studies of the oxidation of alkenes and alcohols will be discussed.

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Abstracts, Continued

77. New Water Soluble Gold(I) Compounds and Their Application in C-C Coupling Reactions

Benelita T. Elie, Tasmin Chowdhury and Maria Contel, Brooklyn College and the Graduate Center, The City University of New York, Brooklyn, NY

Catalyzed carbon-carbon couplings are very important in organic synthesis since the final products are used as intermediates for polymers, natural products and bioactive compounds. The preparation of recoverable and recyclable catalysts for such couplings is of much interest in green chemistry. The area of gold homogeneous catalysis have experience an enormous expansion in the last 5 years.¹ Recent results in this field have brought much interest in the study of gold complexes in different catalytic processes as well as the study on the reaction mechanisms and the nature of the catalytically active species.² Examples of recoverable and recyclable gold compounds in homogeneous catalysis are still scarce.³

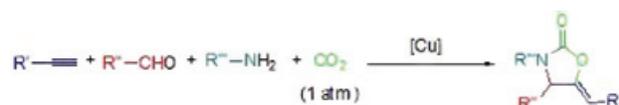
We present here the synthesis of new water soluble gold(I) compounds and their application in the formation of C-C bonds in biphasic systems. Gold(I) compounds of the type $[\text{AuCl}(\text{PR}_3)]$ and $[\text{Au}(\text{PR}_3)_2]\text{PF}_6$ with basic water soluble phosphines of the type $[\text{PR}(\text{C}_6\text{H}_4\text{SO}_3\text{Na})_2]$ or $[\text{PR}_2(\text{C}_6\text{H}_4\text{SO}_3\text{Na})]$ (R = Me, nBu, Cp) have been prepared and characterized. They have been evaluated in Shonogashira and Suzuki cross-coupling of alkynes or arylboronic acids. Results on the recoverability and recyclability of the gold compounds will be discussed as well.

References: (1) Nolan, S. P. *Nature* 2007, 445, 496. (2) Hashmi, A. S. K.; Hutchings, G. J. *Angew. Chem. Int. Ed.* 2006, 45, 78096. (3) For example: Lantos, D.; Contel, M; Larrea, A; Sazbo, D; Horvath. *QSAR Comb. Sci.* 2006, 25, 719.

78. Copper-Catalyzed Synthesis of Oxazolidinones Via Four-Component Coupling Between Aldehydes, Amines, Alkynes, and Carbon Dioxide

Woo-Jin Yoo and Chao-Jun Li, McGill University, Montreal, QC, Canada

With petroleum as the major source of our chemical feedstock, there have been calls for alternative sources due to diminishing levels of this non-renewable resource. Carbon dioxide has the potential to be an excellent C1 feedstock due to its cost and availability. With our interest in developing multi-component reactions, we wish to report to a simple and efficient synthesis of oxazolidinones through a copper-catalyzed coupling of aldehydes, amines, terminal alkynes under atmospheric pressure of carbon dioxide.



79. Properties That Stabilize Proteins to Enzymatic Attack

Li Zhuo and Justin R. Barone, Virginia Tech, Blacksburg, VA

Proteins are promising materials for biomedical and renewable polymers applications. One important property is the stability of the protein in the presence of degrading enzymes during bioresorption or biodegradation. In this study, we degraded proteins corn zein, egg albumin, feather keratin, lactalbumin, and wheat gluten under simulated composting conditions. The proteins had different molecular weights, polarity, secondary structures, and varying amounts of inter-molecular cystine bonding. From the biodegradation behavior as a function of time, four key behavioral features of the biodegradation were found: t_{lag} (lag time), t_{stop} (time at which biodegradation stopped), D_i (initial biodegradation rate), and D_{ss} (steady-state biodegradation rate). It was observed that D_{ss} and t_{stop} depended strongly on cystine bonding, polarity, and α -helix content of the protein. Cystine bonding stabilizes the structure against enzymatic attack. More polar proteins allow enzymes to be

transported in by water and provide sites for the enzymes to anchor. α -helices are compact structures where the C- and N-terminal regions of the peptide bond are shielded by the amino acid side groups, thus inhibiting enzymatic attack. Understanding of these features allows for the synthesis and formulation of protein-based materials with controlled bioresorptions or biodegradations based on the type of molecular structure built into the material.

80. Diesel Engine Exhaust and Endocrine Disruption

Leo Petrilli, Private Citizen, Windsor, ON, Canada

The Canadian Federal Government forecasts over the next 25 years, the province of Ontario's population will increase from just over 12 million to 18 million. Commercial truck traffic is expected to double in the next twenty years. In the border community of Windsor Ontario/Detroit Michigan this will equate to 50,000 trucks a day. Immediate concerns are the effects of diesel engine exhaust on the population—specifically cancer, asthma, respiratory ailments, endocrine disruption, and as the exhaust ends up in smog, ozone, greenhouse gases, global warming and climate change. This discussion is concerned with the suggestion that the chemicals in diesel engine exhaust are contributors to endocrine disruption. The suggestion is that more females than males will be born; there is lots of science that this possibility does exist in fish and wildlife.

The fact that the way the world has chosen to ship freight, specifically by truck, has brought about a significant increase in the amount of pollution. These chemicals are persistent organic pollutants; they contain dioxins, furans, and several chemicals such as benzene, lead, cadmium, and toluene, which are all suspected, probably, or known to be carcinogenic. These chemicals are ending up in the air, water and food chain, especially with indigenous peoples.

The chemicals found in Diesel Engine Exhaust, are similar to chemicals in tobacco smoke, pesticides, herbicides and insecticides. Science needs to discuss and advance this knowledge in order to develop safer fuels.

Is it possible that environmental contaminants are affecting the ability of sperm to survive and contribute to the fertilization process in nature and humans? If this is indeed a fact, then it would make sense that the egg would do everything it had to for survival. This might explain why there are more females in affected populations.

81. Synthesis of Highly Fluorescent Gold Nanoparticles for Sensing Mercury(II)

Huan-Tsung Chang and Chih-Ching Huang, National Taiwan University, Taipei, Taiwan

We have created series of novel, water-soluble, alkanethiol-AuNPs whose fluorescence wavelength is tunable through modification of the chain length of the alkanethiols. The highly fluorescent alkanethiol-AuNPs, such as the 11-MUA-AuNPs, are easily purified and are capable of sensing mercury (II) ions based on fluorescence quenching through mercury (II)-induced aggregation of AuNPs. The sensitivity of the 11-MUA-AuNPs toward mercury(II) was high (LOD = 5.0 nM), with remarkable selectivity over other metal ions in aqueous solution.

82. Environmental Impact of the Two Process for Pseudoboehmite Obtention Using GCES Software

Gabriel Camargo¹, Juan Carlos Moreno², Juliana Serna¹, Joaquin Tirano¹ and Hugo Martin Galindo³, (1)Universidad de los Andes, Bogota, Colombia, (2)Universidad de los Andes, Bogotá, Colombia, (3)Universidad Nacional de Colombia, Colombia

Al_2O_3 is obtained from pseudoboehmite (AlOOH); this precursor can be produced by sol-gel method when Aluminum and Isopropilic alcohol are in contact. Two different catalysts were used (Hgl and sublimed Iode) in order to carry out AlOOH synthesis. Characterization were performed by

XRD, TGA, and BET analysis. The environmental impact in pseudoboehmite (AlOOH) synthesis was investigated. Experimental results were compared with simulation using Green Chemistry Expert System. Textural characterization showed no effect respect to process. Sublimed Iode catalyst indicated that its environmental impact is smaller.

83. Water Purification Using Simplified Solar Distillation Process

Mohammad Musaddaq¹, Shyam Shukla¹, Alka Shukla² and Kenneth Dorris¹, (1) Lamar University, Beaumont, TX, (2) Southeast College, Houston, TX

The news is everywhere that the consumable water resources of this planet are on a serious decline. The efforts are being focused on how to conserve this precious resource of nature around the globe. Out of all the efforts taken, the reuse or recycling of the wastewater are the most phenomenal. To reuse the wastewater various methods are being adopted around the globe and out of these methods many are done on commercial basis, and come with a heavy price tag attached to them. At Lamar University, as part of our Green Chemistry Initiative we have worked with various low cost, readily available, low-tech waste materials to remove metal ions from water. These waste materials often comprise of sawdust or crab shells. In this study we will show a different method of purifying wastewater using solar distillation technique. In this poster we plan to show the methodology, objective, equipment and results obtained from the experiment. We will also show the adaptability of this method in remote places where not many options are available, specially the under-developed countries.

84. Synthesis of a Coordinated Ionic Liquid-(C₄H₉)₄NBr•C₆H₁₁NO

Dishun Zhao, Xiaolei Bao and Tong Wu, Hebei University of Science and Technology, Shijiazhuang, China

Under microwave irradiation, caprolactam and tetrabutyl ammonium chloride as raw material, synthesized a new coordinated ionic liquid-(C₄H₉)₄NBr•C₆H₁₁NO. The effects of reaction time and microwave power to the results were studied. The structure of the compound was characterized via IR. To find the thermal stability range the compound was detected using TGA-DTA. The results indicated that when microwave power is 210W and reaction time is 90s the coordinated ionic liquid had the best properties. The pH value and the conductivity of the compound was 8.9 and 573λ S•cm⁻¹ respectively at 20°C. Compared the spectra of IR of raw materials and product, we found there were new absorption peaks in the product, which showed that the product was not a simple mixture but a new coordination compound. Via TGA-DTA pattern, we obtained that this coordinated ionic liquid can be a stable existence from room temperature to about 250°C.

85. Green Gates to Solid Waste Management in a Chemistry Laboratory

S. Bhanumati, Reader, New Delhi, India

Education needs to be dynamic and adoptive to the changing needs and priorities, while simultaneously providing an arena of freedom to the young innovative and questioning minds. Gradually declining numbers of pupils opting for basic sciences is indeed a disturbing trend. For reversing this trend and for tapping the younger talents science education should be made simpler through practical training right from a primary level itself.

While more and more sophistication in analytical and synthetic techniques to make a subject like chemistry greener is gaining momentum, for a host of well defined reasons in developing countries, simpler strategies involving least wastage, recycling, reusing and reclaiming need to be explored.

The present poster highlights the use and applications of some workable green demonstrations, involving the solid waste generated in a chemistry laboratory.

Melting points have been determined using solid substances as bath as against conc. H₂SO₄, liquid paraffin, etc.

The filter paper shreds (raw and virgin) left after cutting circles have been converted to a pulp being rich cellulosoic and water retaining is ideally suited as beds for growing edible mushrooms.

Recycling of secondary raw material is an important part of green chemistry. Used carbon sheets have been used for filtering hot solutions, for conserving heat, to protect light sensitive chemicals, reagents and reactions.

Glass is an equally important solid waste. Reengineering of broken glass items to useful alternatives has been encouraging. Several examples are cited and illustrated.

Fly ash, a thermal power plant waste along with the other lab generated waste is being put to use on various fronts.

All these ideas projected here comply with the green principles and are worth attempting for the survival of chemistry especially under stringent conditions in terms of grants, natural resources (water), energy (electricity), equipments and glasswares.

86. Comparison of "Green" Concentrate and Ready-to-Use Products

George R. Thompson, Chemical Compliance Systems, Inc., Lake Hopatcong, NJ, Chuck A. Hodge, Ecolab Research Center, Eagan, MN and Cayce Warf, Ecolab, Redmond, WA

Industry recognizes that "green" products are good business. They reduce pollution during manufacture and/or disposal. They reduce worker exposure to hazardous product constituent chemicals. And increasingly, they improve the bottom line. This triple bottom line accounting practice is rapidly becoming the standard for responsible businesses.

As a step in this direction, Ecolab has utilized the "Green" Product Compliance Analytical System (GP-CAS), from Chemical Compliance Systems, Inc., with its chemical-based 43 ecological, health, and safety criteria to evaluate 12 automatic dish, housekeeping and laundry product concentrate and ready-to-use (RTU) formulations for their "greenness." We also evaluated three solvents as concentrates and dilutions. These analyses indicated that GP-CAS is sufficiently sensitive to document improved "greenness" for RTU formulations, when compared to their equivalent concentrates. A similar "green" differentiation occurred with the three solvent concentrates and their dilutions. Clearly, the "greenness" of a formulation is affected by its concentration. "Green" scores calculated for these formulations by GP-CAS were sufficiently wide to allow measurement of continuous improvement in "greenness." These results emphasize the importance of product acquisition decisions being "risk-based," instead of "hazard-based." The availability of alternative constituents within GP-CAS makes this system equally valuable for product design and for product evaluation.

87. Web-Based Systems That Provide Triple Bottom Line Accounting

George R. Thompson, Chemical Compliance Systems, Inc., Lake Hopatcong, NJ

Triple bottom line accounting (also known as "People-Planet-Profit", "environmental-social-economic," "TBL," or "3BL") utilizes an expanded spectrum of data elements, criteria, and values for measuring organizational success. A commitment to this level of social responsibility requires commitment to some form of TBL reporting. Centralized databases utilized by standardized and integrated Web-based analytical compliance systems greatly facilitate migration to this level of organizational commitment—beyond "green" to "sustainability." Environmental accounting can include ecological, biobased,

Abstracts, *Continued*

and recycling product and process analyses. Social values can be enhanced by reducing employee and neighborhood health and safety impacts. Economic improvements can be achieved by quantitatively identifying product and process liabilities and assets, and then wisely choosing management options that minimize liabilities and maximize assets. Implementation of an ISO 14001 environmental management system that quantitatively tracks material/product acquisition, product/process development, and product/process wastes, in light of “green” chemistry principles, will effectively accrue improvements in all three elements of the triple bottom line.

88. Green Engineering and Zero Emission: New Strategies for ISO 14001 Environmental Management System

Omid Tavakoli, Osaka Prefecture University, Osaka Prefecture, Japan

Recently, due to accelerating industrial developments and changes in human lifestyles and activities, increasing waste disposals from various local industries and households pose a grave threat to the environment. Since ISO 14001 is a main reference to evaluate environmental management system, which finally improve all environmental aspects especially in industrial level, any new policy, main legislation or requirement in this subject should be linked to ISO structure. Two important and main requirements which have been gaining more attention of late are green engineering and zero emissions. Both these new aspects influence the improving environmental design from the traditional approach to the new paradigm which is based on the dramatically reduce the environmental impact of hazards. Green engineering offers a powerful set of practical tools to minimize generation of pollution at the source and risk to human health and environment, and then can function well within the ISO 14001 structure. Moreover, zero emissions represent a shift from the traditional industrial model in which wastes are considered the norm, to integrated systems in which everything has its use. Zero emission not only has direct influence on the environment but also will lead to greater efficiency and greater growth in the economy. The application of these aspects is especially important when dealing with extremely hazardous materials. This focus on green engineering and zero emission which provide new design at the source and during process, serves as a new adjunct to the traditional waste management, recycling, reuse and energy issues typically addressed in ISO 14001 programs.

89. Analysis of the Environmental Impact of Phenol Wastewater Treatment Processes

Enrique A. Campanella, Instituto de Desarrollo Tecnológico para la Industria Química (UNL—CONICET), Santa Fe, Argentina and Guillermo A. Ontiveros, Universidad Nacional del Litoral, Santa Fe, Argentina

This work studied environmental evaluations of wastewater treatments of a residual stream contaminated with phenol. A process simulator was used in order to design four alternative treatments: liquid-liquid extraction, supercritical extraction, catalytic oxidation and supercritical oxidation. On the other hand, the Waste Reduction Algorithm (WAR GUI 1.0, USEPA) was chosen to determine potential environmental impacts for each treatment process design. The information obtained in this work is used to determine which alternative is more environmentally friendly to remove phenol, and to find an environmental metric to carry out preliminary designs of environmentally friendly processes. To evaluate environmental behavior a three-step process was used. First, a limited number of alternatives were generated from a basic scheme. Subsequently, simulations of each process were worked out by a chemical process simulator and optimal operational conditions were chosen. As last step, influence of different environmental index of each analyzed process was weighted qualitatively and quantitatively. Once collected all necessary information, a critical evaluation of data was carried out and diverse observations were extracted. First, total generation rate of PEI (Potential Environmental Impact) presents negative values in all cases, which shows that processes are environmental friendly. In addition,

in liquid-liquid extraction and supercritical extraction, recovered phenol may be recycled as product and any waste is generated. Second, the impact generated by energy production is lower than the benignity of the whole process even when the worst energy source (coal) is chosen. Finally, as complex calculations were done process simulation has been essential to determine thermodynamic behavior of all analyzed processes and to select their best operational conditions.

90. Alcohol Cross-Coupling Reactions Catalyzed by Ru and Ir Terpyridine Complexes

Dinakar Gnanamgari, Yale University, New Haven, CT

Primary alcohols can be coupled with secondary benzylic alcohols by an air-stable catalytic system involving terpyridine ruthenium or iridium complexes, the products being coupled alcohols (Ru) or ketones (Ir).

91. Environmentally Friendly Approach to Microwave-Assisted Organic Synthesis of Imidazo[1,5- α]Pyridines

Anastasia S. Lyons, Clark Atlanta University-USDA/Forest Services/Forest Products Laboratory, Atlanta, GA, Roger M. Rowell, University of Wisconsin, Madison, WI and Xiu Ren Bu, Clark Atlanta University, Atlanta, GA

Imidazo[1,5- α]pyridines are a novel class of ligands that have gained recognition for its biological and medicinal applications. Recently, these ligands have been covalently incorporated into organic-inorganic hybrids as a means to remove heavy metal ions from water. Traditionally, the synthesis of imidazo[1,5- α]pyridines was limited to low yielding multi-step reactions, expensive and harsh reagents, and excessive reaction times. Here, we employ time and energy efficient microwave irradiation with milder reagents to synthesize a class of imidazo[1,5- α]pyridines. We hope to obtain higher yields and develop more environmentally friendly reaction conditions.

92. The Development and Application of Room Temperature Ionic Liquids

Xiaomei Hu, Aston University, Birmingham, United Kingdom

There is an urgent need to develop alternative solvents and technologies for synthetic chemistry due to the increasing need for protecting the environment. Room temperature ionic liquids (RTILs) as “green solvents” which belong to green chemistry have gained wide popularity in recent years for their increasing applications in the areas of synthetic and biological chemistry as they possess a number of interesting properties, especially their lack of vapor pressure and lack of flammability, a widely accessible temperature range and ease of reuse. Therefore they are considered to be environmentally friendly reaction mediums. Moreover, their properties such as solubility, density and viscosity can be adjusted to suit the requirements simply by changing the nature of the cations or anions. Due to all the benefits, RTILs are applied in many organic reactions.¹

In our lab, different methods were applied to synthesis various kinds of ionic liquids such as ionic liquid [BMIM]Cl, [BMIM]Br or room temperature ionic liquid [BMIM]BF₄, [MOEMIM]⁺OMs⁻ etc. We also synthesized some new class of ionic liquids. In addition, for the application of RTILs, some organic reactions were investigated in RTILs. For the first time, [BMIM]BF₄, [BMIM]PF₆ were as both catalyst and solvent to promote organic reactions. All these experiments indicated that RTILs have a great potential as alternative solvents in synthetic chemistry.

Furthermore, Nucleoside chemistry is an important research area in drug discovery. Various chemical modified nucleosides, oligonucleotides have therapeutic activities.²⁻³ However, one big problem is the poor solubility of these nucleoside compounds in the common organic solvents. RTILs such as [MOEMIM]⁺OMs⁻ have a good solubility to these nucleosides. Here, some

modified thionucleosides with potential pharmaceutical applications have already been synthesized in several RTILs with high yields. These chemicals will then be investigated for their anti-cancer properties.

93. 2008 HANCOCK AWARD RECIPIENT High-Throughput, Low-Waste Synthesis of Well-Defined Gold Nanoparticles In Microcapillary Flow Reactors

Lallie McKenzie and James Hutchinson, University of Oregon, Eugene, OR

As the focus on novel nanoparticles (NPs) changes from fundamental research to widespread use in applications, large-scale synthesis routes become increasingly important. In particular, production methods that provide substantial yields of high-performance NPs and simultaneously reduce the environmental impact of these processes are in demand. Although current methods are effective for research-scale synthesis, yields of desired materials are low, large amounts of waste are produced, and reaction scale is limited. The synthesis of NPs in flow systems with microscale dimensions has been shown to increase control of NP pore size and lead to improved products. Along with these benefits, we demonstrate that flow synthesis in a simple, versatile microcapillary reactor can lead to improved NP production methods that are suitable for large-scale operations. We investigated the synthesis of subnanometer gold particles and report the development of new production methods that not only dramatically improve the uniformity of the NPs but also significantly increase the efficiency and throughput of their production. Key results include direct synthesis of monodisperse NPs, a four-fold increase in yield, a hundred-fold increase in production rates (up to 8 g/hr), and an 80% reduction in solvent waste. This work demonstrates that integrating the principles of green chemistry into the development of new nanomanufacturing processes can effectively reduce environmental impacts and enhance the economic and technological viability of these approaches

94. Photo-Induced Solid State Absolute Asymmetric Synthesis In Nanocrystalline Suspensions

Farnosh Family and Miguel Garcia-Garibay, University of California, Los Angeles, CA

Solid state photochemistry has tremendous potential as a green chemistry methodology to obtain enantiomerically enriched chiral products. However, further improvements can be made through the use of nanocrystalline suspensions in environmentally benign water. By reducing the size of the crystals to about 200 nm and starting from chiral crystals, we have improved the enantiomeric excess of several photochemical absolute asymmetric reactions. One reaction examined by this process is the di-g methane rearrangement of a dibenzobarralene ester which can crystallize in a chiral space group. Previous reports of the reaction showed a maximum % ee at 30% conversion where the reaction stops due to the crystal lattice breaking down. In this study, we found that grinding chiral crystals and creating suspensions in water created a 65% ee at 85% conversion. Another example is the electrocyclization of 2-pyridinone derivatives. Meta-substitution on the benzyloxy attached at the 4 position of the 2-pyridinone created crystals that packed in chiral space groups. Using solely the chiral information in the crystal, an enantiomeric excess was created.

95. Purification Strategies Via Greener Methods for Reductive Amination Reactions Using Resin-Bound Agents

Hephzibah J. Kumpaty, University of Wisconsin-Whitewater, Whitewater, WI

Amine synthesis is an important reaction in drug discovery. One of the key methods for the preparation is via Reductive amination of carbonyl compounds. Reductive amination proceeds through the formation of an imine intermediate

upon reaction of a carbonyl compound with primary or secondary amine and is followed by in situ reduction to an amine of higher order. The use of polymer-bound reagents and scavengers provides an attractive alternate approach for integrated organic synthesis and benign purification methods, as the reaction byproducts and excess substrates can be selectively removed from the reaction mixture by simple filtration, thus eliminating the need to use traditional column purification method. We have used polymer-bound reagents to streamline work-up and purification steps in reductive amination reactions. Following reductive amination, crude products were purified by the addition of a catch and release MP-TsOH resin. For catch and release purification, the reaction mixture is filtered and added to MP-TsOH column. This quantitatively 'catches' the product amine by forming a salt on the resin, allowing suitable removal of non-basic byproducts and starting materials by washing with small amounts of organic solvents. Selective 'release' of the amine is then effected by addition of a methanolic ammonia solution to the resin.

96. Using a Capillary-Based Microreactor Screening System in Green Analytical Chemistry: Throughput Study

Lei Hong and Stephen Weber, University of Pittsburgh, Pittsburgh, PA

The microreactor confers many advantages over conventional scale chemistry, including enhancement in heat and mass transfer, high surface to volume ratio, ease control of concentration gradients, and reduced exposure to toxic and hazardous materials, which inherently make microreactor green the analytical chemistry.

Although to date the majority of microreactor systems are built up on a chip platform, they are impractical for slower reactions. We have devised a parallel approach in which many boluses of reactants are injected serially into a capillary-based microreactor. The reactions, which may take hours, occur in parallel. This system allows us to conduct the research on screening for catalysts and reaction conditions with high-throughput.

A mathematical model has been established in order to predict the maximum throughput via adjusting the process parameters, such as capillary dimension, flowrate, and reaction time. Lanthanide triflate-catalyzed allylation reactions of benzaldehyde with tetraallytin were used as the model reactions. Common Lewis acids are very sensitive to the presence of water, however, lanthanide triflates can function as Lewis acids in aqueous solutions. In addition, lanthanide triflates can be easily recovered after the reaction and reused without losing activity. These unique properties have made lanthanide triflates extremely attractive using as catalysts in green chemistry. The calculation showed that high flowrate and small inner diameter of capillary reactor favor higher throughput. Using a continuous flow, the maximum throughput of the microreactor is able to reach 16 reactions per hour for a two-hour reaction using a 75µm ID capillary and 20µL/hr flowrate.

97. Chitosan Based Scaffolds by Lyophilization and sc CO₂ Assisted Methods for Tissue Engineering Applications: A Benign Green Chemistry Approach

Kumari Rinki and Pradip Kumar Dutta, Motilal Nehru National Institute of Technology, Allahabad, Allahabad, India

Chitosan scaffolds with possible tissue engineering applications were synthesized and those treated under lyophilization and supercritical carbon dioxide (sc CO₂). 1% Chitosan solution in aq. acetic acid was treated with 37% formaldehyde solution; the resulting hydrogels were subjected to solvent-exchange before the final treatment procedures. Their morphology, pore structure, and physical properties were characterized by FTIR, NMR, thermal analysis, scanning electron microscopy, X-ray diffraction and porosimetry analysis. The sc CO₂ treated scaffolds showed much greater porosity and surface area in comparison to the lyophilized one. The lyophilized and sc CO₂

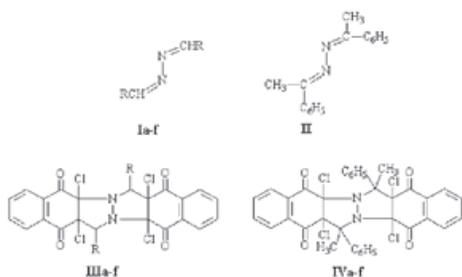
Abstracts, Continued

treated both kinds of scaffolds have antibacterial properties. The sc CO₂ assisted chitosan scaffold under green chemistry approach is highly pure and from hygienic point of views it is an ideal material for biomedical applications.

98. Synthesis of Some New Bispyrrolidine Derivatives for Biological Interest (Part V)

Representatives of this system belong to a class of biological active compounds and at the same time are excellent starting materials for developing a new type of biological active compounds.

Thermally induced crisscross¹⁻⁵ cycloaddition of azines I and II (1 mole) in presence of 2,3-dichloro-1,4-naphthoquinone (2 moles) afforded the adduct III and IV respectively in one-pot reaction. The molecular structure of the products is reported and discussed. The processes for obtaining the title compounds reduce the use and generation of hazardous substances.



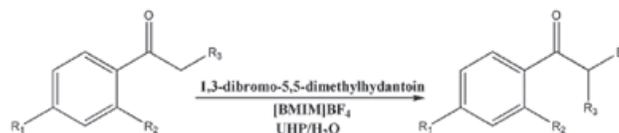
I,III a) R = -C₆H₅, b) R = -C₆H₄-*p*-OCH₃, c) R = -C₆H₄-*o*-OH,
d) R = -C₆H₄-*p*-Cl, e) R = -CH=CH-C₆H₅, f) R = -C₄H₉

References: (1) Wagner-Jauregg, Ber., 63, 3224 (1930). (2) Van Alphen, Rec. Trav. Chem., 61, 892 (1942). (3) Amal Sabet Yanni, 16th International Conference on Physical Organic Chemistry, San Diego, CA, USA, August 4-9 (2002). (4) Amal Sabet Yanni, Polymer Networks 2004 Conference, Bethesda, Maryland, USA, August 15-19 (2004). (5) Amal Sabet Yanni, 10th Annual Green Chemistry Conference, Washington DC, USA, June 24-29 (2006).

99. A Mild and Environmentally Friendly α -Bromination of Ketones in Ionic Liquid Using 1,3-Dibromo-5,5-Dimethylhydantoin (DBDMH) and UHP in H₂O

Soon-Uk Chang and Jong Chan Lee, Chung-Ang University, Seoul, South Korea

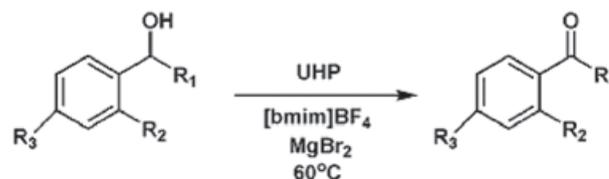
Evolution of environmentally friendly synthesis is a paramount goal of the present day organic chemistry. In recent years, ionic liquids have been acknowledged as green alternatives to the toxic and volatile organic solvents for various chemical reactions. Bromination of organic compounds is one of the important synthetic implement in organic syntheses. The drawbacks of many known bromination methods associated with the use of organic solvents and toxic reagents lead us to develop greener bromination systems. In this context, a new environmentally friendly bromination protocols has been developed. In our work, an efficient and selective α -bromination of ketones by use of 1,3-dibromo-5,5-dimethylhydantoin (DBDMH) and UHP in H₂O in ionic liquid at 50-60°C is smoothly achieved. Bromination with 1,3-dibromo-5,5-dimethylhydantoin (DBDMH) as a source of bromine cation have been accomplished a mild and environmentally benign UHP in H₂O and provides selectively bromination in excellent yields in the presence of catalytic ionic liquids.



100. A New Method for Oxidation of Benzylic Alcohols Using MgBr₂/UHP in Ionic Liquid

Hee Joong Park and Jong Chan Lee, Chung-Ang University, Seoul, South Korea

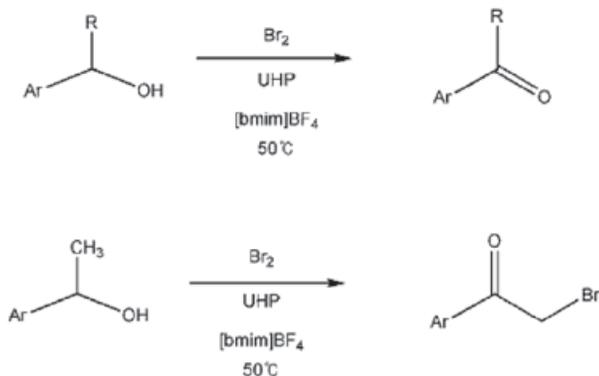
The transformation of benzylic alcohols to carbonyl compounds is one of the most fundamental reactions in organic synthesis. Various methods have been developed for the oxidation of benzylic alcohols to the corresponding benzaldehydes or ketones. However, the majority of known methods commonly have one or more disadvantages such as difficulty in manipulation, long reaction times and utilization of toxic reagents. Therefore, it is still desirable to develop a new efficient oxidant with properties of high stability and low toxicity ready availability for the benzylic oxidations. In recent years, ionic liquids have been acknowledged as green alternatives to the toxic and volatile organic solvents for various chemical reactions. The urea hydrogen peroxide complex [CO(NH₂)₂H₂O₂, UHP] considered as oxidation reagents of choice due to its safe and environmentally friendly nature. In recent years, UHP has proved to be effective in solid state reactions, both under heating or microwave irradiation, so becoming an interesting eco-friendly reagent. Effective oxidation reactions of primary and secondary benzylic alcohols into the corresponding benzaldehydes or ketones have been accomplished using magnesium bromide (MgBr₂) and urea hydrogen peroxide (UHP) in [bmim]BF₄ ionic liquid.



101. Simple and Efficient Oxidation and α -Bromination of Benzylic Alcohols by Using Br₂/UHP in Ionic Liquid

Jimi Kim and Jong Chan Lee, Chung-Ang University, Seoul, South Korea

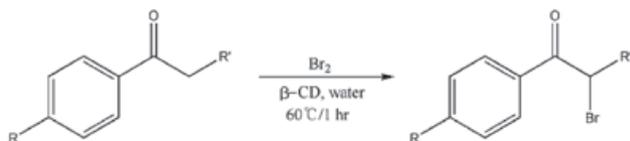
The oxidation of alcohol to carbonyl compounds has been recognized as a fundamental organic transformation in organic synthesis. However, such transformations have been generally performed with environmentally hazardous inorganic oxidants, notably chromium(VI) reagents, pyridium dichromate and manganese reagents. Therefore, it is still desirable to develop a new efficient oxidation method for benzylic alcohols with properties of high stability and low toxicity. In these viewpoints, we investigated the feasibility of bromine/UHP in ionic liquid as green oxidation system. A mixture of aromatic ketones and bromine was heated and stirred in the presence of urea hydrogen peroxide in [bmim]BF₄ ionic liquid. The carbonyl compounds were obtained within 1-3 hr at 50°C in high yield (70-90%). In cases of secondary alcohols, twice amount of bromine were required to give α -bromo ketones. We have developed new alcohol oxidation conditions which are simple, mild, easy to handle.



102. New Method for α -Bromination of Ketones Using Br_2 and β -Cyclodextrin in H_2O

Seul Lee, Chung-Ang University, Seoul, South Korea and Jong Chan Lee, Chung-Ang university, Seoul, South Korea

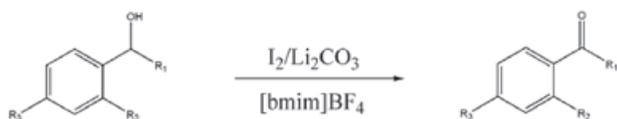
Direct conversion of carbonyl compounds into α -halocarbonyl compounds is very important synthetic transformation that has been received considerable attention. A mixture of aromatic or aliphatic ketones and bromine was heated and stirred in the presence of β -cyclodextrine in water. The monobromoketone was obtained exclusively within 1 hour at 60°C in high yields (70–90%). In this work, the reactions have been carried out without use of any toxic organic solvent and metal based catalyst and strong acid.



103. New Method for Oxidation of Benzyl Alcohols Using Ionic Liquid

Seungbae Lee and Jong Chan Lee, Chung-Ang university, Seoul, South Korea

Rather than striving to minimize human exposure to and environmental release of hazardous organic solvents, green chemistry seeks to replace hazardous solvents with alternative solvents or reaction media presenting reduced health risks and environmental impact. In this viewpoint, one of the most interesting features of $[\text{bmim}]\text{BF}_4$ is its ability to be a powerful alternative to the other hazardous organic solvents. In our work, we thought that more efficient, environmentally benign method in $[\text{bmim}]\text{BF}_4$ was necessary and use of iodine should overcome one or more disadvantages shown in other conventional oxidation methods. In this respect, we studied the oxidation of benzyl alcohols by using $\text{I}_2/\text{Li}_2\text{CO}_3$ in $[\text{bmim}]\text{BF}_4$. In this work, the oxidation reactions of primary benzylic alcohols with $\text{I}_2/\text{Li}_2\text{CO}_3$ at 60°C gave excellent yield of benzaldehydes. After I_2 and Li_2CO_3 were mixed in $[\text{bmim}]\text{BF}_4$. In cases of secondary benzylic alcohols the corresponding ketones were obtained in yields.



104. Fluorinated Polymeric Binap Ligand for Asymmetric Hydrogenation in sc CO_2

Ozlem Erdem and Bilgehan Guzel, CU Science and Letters, Adana, Turkey

In the past decades, the attachment of homogeneous catalysts to soluble polymer supports has been attracting considerable attention owing to its potential combination of the advantages, and minimization of the disadvantages, of homogeneous and heterogeneous catalysis¹.

Here, we report use of polymeric chiral diphosphine ligands for asymmetric hydrogenation. BINAP was chosen as a model ligand for this study, since it is probably the most versatile and effective ligand among all the chiral phosphine ligands which have been studied for asymmetric catalysis^{1,2}. The chiral polymeric BINAP ligands were synthesized in 71% yield by condensation of the 6,6'-diaminoethyl-BINAP with terephthalaldehyde in N-methyl-2-pyrrolidone (NMP).

The ligands were characterized ¹H, ¹⁹F and ³¹P NMR. The molecular weights of polymeric ligands were determined by gel permeation chromatography (GPC). Solubility studies in sc CO_2 were performed at the conditions of 343°K, 2300 psi pressure. Complexed with rhodium it gives 85% conversion and enantioselectivities from 62% for the hydrogenation of α -ketoester. Hydrogenation was carried out in 0.032 mol-L⁻¹ (0.063 mmol of ligand) solution of sc CO_2 under following reaction conditions: Substrate/catalyst = 200 (molar ratio); H_2 pressure 6,76 x 10⁶ Pa., CO_2 pressure 2300 psi. Conversion and ee were determined by chiral GC analysis.

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105. 2008 BREEN FELLOWSHIP RECIPIENT: Integration of Green Chemistry Experiments In Chemistry Teaching Methods Course

Mageswary Karpudewan, Zurida Hj Ismail and Norita Mohamed, University Sains Malaysia, Penang 11800, Malaysia

Agenda 21 of UNESCO's Decade of Education for Sustainable Development (2005–2014) is centered on man and calls for humankind to change behaviors to attain sustainability. Education plays a critical role in realizing sustainable development and promoting the capability of the people to address environmental issues towards improving the quality of life for the present and future generations. One approach that could be adopted to attain this goal is through greening the chemistry curriculum particularly the practical work. Green chemistry can contribute to sustainable development through application and extension of its 12 principles. The interdisciplinary nature of green chemistry which embeds economical, environmental and societal dimension is a student centred deep learning approach. However, the success of green chemistry depends on the training and education of a new generation of chemists. Hence, there is a need to educate our teachers with the principles of green chemistry and how to teach green chemistry. Accordingly, this paper reports on the implementation of green chemistry as a laboratory based pedagogy in the chemistry teaching methods course for pre-service teachers. The integration of green chemistry into the science teacher education program is considered important as it possesses the potential to influence many future teachers and ultimately many students as well.

Abstracts, *Continued*

106. Greening the Undergraduate Organic Chemistry Laboratory through the Biginelli Reaction

Lois Ablin, Oral Roberts University, Tulsa, OK

The Biginelli reaction is an acid-catalyzed reaction of urea, an aromatic aldehyde, and a beta-keto ester in a single reaction vessel to produce dihydropyrimidinones, compounds of interest in medicinal chemistry. Procedures have been developed to increase the greenness of this reaction and produce the products in good yield.

107. Project Green at the University of Pittsburgh

Lawrence B. Friedman, University of Pittsburgh, Pittsburgh, PA

Project Green at the University Pittsburgh is a one-year effort to incorporate the principles of Green Chemistry into the culture of a large, diverse, Ph.D.-granting chemistry department. The project is funded by the National Science Foundation through a Discovery Corps Fellowship to the author.

The project has a research component as well as an education/service component. The research focuses on the capture of carbon dioxide using a set of novel, ionic liquid-based polymers. These polymers are being designed, synthesized and characterized in the Department by a team of undergraduates in collaboration with a senior member of the faculty and the author. This research team has established a relationship with the nearby National Energy Technology Laboratory (NETL) and using facilities at NETL will evaluate the effectiveness of the polymers for separation of carbon dioxide from gas streams and flue gases that are produced in coal-burning electric power plants.

The education/service component of the project includes teaching a short course on green chemistry and organizing a departmental seminar program that is bringing leaders in green chemistry and chemical engineering to the University to make technical presentations and interact with students. In addition, undergraduates are contributing to the development of green chemistry laboratory projects for mainstream introductory and organic chemistry courses. These students also are involved in outreach with the University's College in High School program and with a local chemical technician training program.

108. The Role of Guided Inquiry and Microscale Chemistry in Green Chemistry

Alka Shukla¹, Shyam S. Shukla², Mohammad Musaddaq², Leena Purohit³ and D. Shukla⁴, (1)Southeast College, Houston, TX, (2)Lamar University, Beaumont, TX, (3)Asish Higher Secondary School, Ahmedabad, India, (4)MNS BED College, Ahmedabad, India

The apocalyptic opinions and views are nowadays abound in the popular media. Part of such view may arise from misconception while other may have sound basis in the science. We may debate this issue but the facts remains that the demands of the global resources are increasing rapidly causing a rapid decrease in the quality of the environment. We all are responsible for creating these problems and we all have to contribute towards the solutions of problems of environmental deterioration. We have laid our focus on academia for at least two reasons. It is at these institutions where our thoughts are shaped which we carry through our lives. Thus we want to develop techniques, material and methods to train people in the issues of "Green Chemistry" around the world. Secondly, in this process we want to improve science education (which we do through peer leading, guided inquiry, etc). We have undertaken a national and international mission through Lamar Outreach Program to achieve both of these goals and in this poster we will describe our mission, methods, and difficulties.

109. Greening up the Synthesis of Aspirin

Kathleen D. Field and Carolyn Supplee, Monmouth University, West Long Branch, NJ

Traditionally aspirin is synthesized by an esterification reaction between the phenolic hydrogen of salicylic acid and acetic anhydride in the presence of a Brønsted-Lowery acid catalyst, sulfuric acid, in the absence of water. If water is present, aspirin is known to undergo a hydrolysis reaction which yields the starting materials.

The synthesis of aspirin is often used as an experiment in general chemistry to demonstrate the concepts of chemical kinetics and equilibrium and to teach students synthetic chemistry skills. Since the reagents used in the synthesis of aspirin and the aspirin product, itself, are colorless, the general chemistry experiment for the synthesis of aspirin is not visually interesting to students. And often times, the reaction does not produce aspirin in high yield or purity. The major impurity that has been identified by infrared spectroscopy and melting point determination is salicylic acid. Salicylic acid can be attributed to the small amount of water in the laboratory equipment causing the reverse hydrolysis reaction.

In order to make the experiment visually more interesting, increase the quality and quantity of aspirin produced and reduce the students' exposure to concentrated sulfuric acid, an alternative procedure for the synthesis of aspirin was developed using a transition metal catalyst. The use of a suitable transition metal catalyst makes the reactions solutions highly colored, produces a high quality of aspirin and allows for the synthesis of aspirin without the use of concentrated sulfuric acid. This study examines the affect of changing the catalyst on the synthesis of aspirin.

110. LCA and EHS Comparison of Biocatalytic and Chemical Pharmaceutical Synthesis: 7-ACA

Concepción Jiménez-González, GlaxoSmithKline, Research Triangle Park, NC, Richard K. Henderson, GlaxoSmithKline, Ware, Hertfordshire, United Kingdom, David JC Constable, GlaxoSmithKline, Philadelphia, PA, Chris Preston, GlaxoSmithKline, Ulverston, Cumbria, United Kingdom and John Woodley, Technical University of Denmark, Lyngby, Denmark

Recognition of the benefits of selective catalysis has resulted in the introduction of a considerable number of biocatalytic reactions into synthetic strategies for potential Active Pharmaceutical Ingredient (API) manufacture. In addition, conventional wisdom typically asserts that there are potentially considerable environmental improvements and cost reduction associated with the use of biocatalysis. However without a rigorous and quantitative comparison between more traditional chemical and newer biocatalytic routes, it remains merely a perceived benefit. The present research intends to fill this gap.

The main goal of this work was to estimate and compare the environment, health, safety and life cycle impacts of two synthetic methods used to produce the API 7-aminocephalosporic acid (7-ACA). The routes under study were a chemical synthetic process and a two-enzyme catalyzed process both starting from the potassium salt of cephalosporin C.

The methodology employed for comparison was a Green Technology Comparison framework previously presented. This method compares EHS performance utilizing GlaxoSmithKline's (GSK) sustainability metrics, and incorporates a life cycle approach. The cradle-to-gate life cycle impact estimations were performed using GSK's Fast Life cycle Assessment of Synthetic Chemistry (FLASCTM) tool and the modular gate-to-gate methodology developed in partnership with North Carolina State University.

Results are presented that compare efficiency, environment, health, safety and life cycle metrics for the chemical and enzymatic routes, both when only looking at the process itself and when accounting for the cradle-to-gate environmental life cycle impacts.

This research represents one part of GSK's ongoing efforts to move towards more sustainable business practices, by investigating novel, greener processes for producing Active Pharmaceutical Ingredients and estimating and optimizing their life cycle impacts.

111. Natural Oil Polythiols and Polyols— a Life Cycle Comparison

Thomas A. Upshaw, William J. Fisher and Eric J. Netemeyer, Chevron Phillips Chemical Co LP, Bartlesville, OK

Polythiols are known to be effective hardening agents for epoxy resins, providing access to low cure temperatures. Polythiols can also be used with isocyanates to produce polythiourethanes and as co-reactants for curing multi-olefinic compounds through thiol-ene chemistry. Novel polythiols derived from soybean oil have been developed by Chevron Phillips Specialty Chemicals and examined for their utility in coatings and adhesives applications. These polythiols offer the additional benefit of sustainability since they are derived from a natural source oil. It is instructive to compare the cradle-to-customer life cycle impacts of mercaptanized soybean oil (MSO) with commercial petroleum-derived polyether polyols and with available natural oil-based polyols. The presentation will include a discussion of the process scope, life cycle methodology and initial life cycle analysis of these products, summarizing various environmental impact factors and weighted BEES scores.

112. Clean and Green: Progress in the Development of Environmentally-Friendly Lubricants

Alan C. Eachus, Independent Consultant, Villa Park, IL

Whether impelled by profit, legislation or altruism, lubricants which are considered to be less environmentally-damaging than their predecessors continue to increase in use. While these products generally demonstrate improved biodegradability and lowered eco-toxicity, and are based largely on "renewable" ingredients, there is not yet complete agreement as to the criteria for such designation, nor regarding the test procedures and resulting data required for inclusion in this category.

While various base fluids have received the most scrutiny as alternatives to mineral oil, appropriate additive packages must be developed for each, as well. Advances in the field continue to be made, based on a variety of factors. Perhaps the most-challenging lubrication application is in an engine crankcase; this environment also provides unique opportunities for indirect lubricant "greenness."

By far the greatest impediment to more widespread adoption of environmentally-benign lubricants is their significantly higher cost over conventional ones. This disadvantage is expected to gradually lessen, based on continuing pressure from the combination of technology advances, legislative restrictions and tax incentives, coupled with the possibility of further increases in crude-oil costs.

113. Automated Ammunition Design for Demil Utilizing Web-Based "Green" Capabilities

George R. Thompson¹, Kevin Kennedy¹ and Tyrone D. Nordquist², (1)Chemical Compliance Systems, Inc., Lake Hopatcong, NJ, (2)U. S. Army Defense Ammunition Center, McAlester, OK

A series of Executive Orders and DoD Directives has created a need for the military to develop "green" munitions—munitions that minimize effects on human health and the environment, and also can be more cost effectively demilitarized at the end of their life cycle. PEO Ammunition and the U.S. Army Defense Ammunition Center (DAC) funded the implementation of the "Green" Munitions Analytical Compliance System (G-MACS) on the World Wide Web.

G-MACS objectively and quantitatively calculates the "greenness" of a munition and its components/parts/ chemicals, including explosives, without delaying the development of new munitions. G-MACS is based upon 43 weighted "green" criteria that encompass ecological, health, safety and regulatory impacts of explosives and other munition chemical constituents. Total "green," or criteria segment, scores can be quantitatively compared for an old and new munition to analyze their relative "greenness," or the scores can be used to rank the "greenness" of a series of equivalent munitions (e.g., grenades), or munition parts (e.g., fuses). "Green" assessments can be performed during the design of a munition, or to evaluate an existing munition. Although G-MACS was implemented to facilitate development of new "green" munitions, it will more frequently be utilized to analyze munitions in use to identify mechanisms to improve their greenness by substitution of less hazardous materials, such as "greener" explosive parts. Additionally, G-MACS can be utilized to create a "Green" Components, Parts, or Energetics Index, that facilitates selection of materials with higher "green" scores during the development of new munitions, or the improvement of munitions in production. G-MACS is currently "live" on the Web. Users who will benefit from the use of G-MACS include purchasing agents, design engineers, ammunition development contractors, environmental/safety/health professionals, program managers, shipping/transportation/ storage personnel, and a variety of munition supervisors.

114. Sustainability Framework for Process and Product Development

Carol English, Cytec Industries Inc, West Patterson, NJ, David Taschler, Air Products & Chemicals, Inc., Allentown, PA and Charlene A. Wall, BASF Corporation, Florham Park, NJ

The Center for Sustainable Technology Practices (CSTP), an industry consortium, has developed a conceptual roadmap that connects the critical corporate functions of a company with major value chain stages and important sustainability considerations. The Business Strategy Alignment and Upstream Supply functions will be highlighted to show both the utility and outcomes of the use of the roadmap in decision making. The Sustainability Roadmap can support organizations that are either interested in integrating new sustainability considerations into their Business or enhancing existing sustainability-related initiatives. The Roadmap is flexible, may be edited, and was developed such that users can customize the tool for use by their specific organization.

115. CleanGredientsSM as a Consensus-Based Tool

Alec Gosse and Topher Buck, GreenBlue, Charlottesville, VA

As the discussion of what defines a "green" chemical or product expands, an information format to capture consensus on this question must itself grow increasingly complex. CleanGredientsSM is a tool to present physical-chemical, human health, and environmental information about chemicals used in the formulation of industrial and institutional cleaning products. It is designed specifically as a vehicle to facilitate discussion of the relative importance of various ingredient attributes in particular contexts and thereby to support product-design decisions across a broad spectrum of perspectives and objectives. Attributes for each ingredient class in the tool are selected by a Technical Advisory Committee convened through an open stakeholder-engagement process that provides a rational, science-based framework to promote the understanding and application of proactive and precautionary design principles. CleanGredients includes metrics to establish requirements for listing and to meet the "DfE Screen," a benchmark established by U.S. EPA Design for the Environment (DfE) Program to identify chemicals in an ingredient class that have the most positive human health and environmental profiles. CleanGredients users gain cost savings and efficiency through new or expanded access to information supporting greener formulation and product design. At the same time, raw materials suppliers benefit from access to a growing market for their greener chemicals, which should stimulate more investment in green chemistry R&D. As the move toward sustainability leads the marketplace to

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embrace an expanded definition of quality that includes environmental and human health impacts. CleanGredients provides information essential to making well-informed decisions.

116. Chemical Product Evaluation and Screening—Tools for Real World Decision Making

Marilyn Johnson, Dolphin Software, Inc., Lake Oswego, OR

When a company endeavors to green the chemicals in their supply chain, a first, critical step is to effectively access and employ information that enables better decision-making. The process starts with knowledge of what kinds of chemicals (and their constituents) are available in today's marketplace. Advanced software tools today can enable companies to leverage chemical product information, specific to their needs. A demonstration of these tools will be provided. These tools are designed to help bring objectivity and clarity to each particular chemical product's health and environmental impacts—information that those who design, buy or use products need to know—and which will provide a basis for company decisions and action. These screening tools help answer questions that support company and customer needs through full product information disclosure and assessment, while protecting confidentiality of ingredient formulation. This neutral third-party platform for the design and deployment of customized product screening was built on a background of 15 years of chemical management software expertise.

117. Pulling down the Barriers: Lessons from Local and International Variations in Green Chemistry Policy

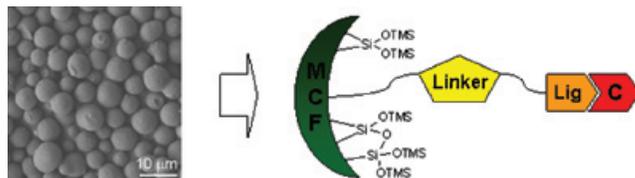
Kira JM Matus, Harvard University, Cambridge, MA

This presentation will examine the variation in the implementation of green chemistry from the policy perspective, with a focus on how local contexts can change the nature and severity of barriers and incentives that impact the implementation of green chemistry. Comparisons across the United States, as well as in other countries, such as China, show that the difference in environmental policy, business climate, intellectual property regimes, educational system, cultural norms and practices and other local factors can have a significant impact on the success of green chemistry. This, in turn, points to some useful lessons for policy makers, members of the business community, researchers and practitioners who seek to advance green chemistry at both the local and global level.

118. Siliceous Mesocellular Foam (MCF) Supported Catalysts for Green Chemistry

Jaehong Lim, Su Seong Lee and Jackie Y. Ying, Institute of Bioengineering and Nanotechnology, Singapore, Singapore

We have developed siliceous mesocellular foam (MCF) as a facile and versatile support material for heterogenized catalysis. This material is attractive for its robust, well-defined pore structure with interconnected, ultra large pores that facilitate diffusion. Catalytic complexes are successfully immobilized on MCF, and easily recycled. By tuning the property of the linker groups and the microenvironment, these heterogenized catalysts were effectively applied towards useful reactions such as ring-closing metathesis (RCM) and asymmetric cyclopropanation. A circulating flow-type reactor has also been developed to circumvent the gaseous byproducts in packed bed reactors for large-scale reaction. Excellent activity and extremely low level of metal leaching were attained with these robust catalysts. These heterogenized catalysts and reactor scheme would facilitate the development of environmentally friendly and more cost-efficient industrial processes.



119. The Use of Transparent Colloidal Titania Sol for Degradation of MTBE and Nitrophenol

Shyam S. Shukla¹, Kenneth Dorris¹, Hardik Shah¹, Mohammad Musaddaq¹ and Richa Shukla², (1)Lamar University, Beaumont, TX, (2)University of Texas Medical Branch, Galveston, TX

The problem of disposal of toxic waste is serious, but the methods currently available are either complex and expensive or may result in generation of some other unwanted material during the disposal. There is a great need for economical and simple methods for disposal and degradation of both organics and inorganics. In our work we have utilized colloidal titania sol prepared by extremely simple means and use them for degradation of various organic compounds. In this presentation we will discuss the property of the "TRANSPARENT" titania sols that we have prepared using Titanium tetrachloride in our lab, and how they have been utilized to photocatalytically degrade MTBE and nitrophenol. MTBE is an extremely persistent pollutant because it is extremely stable to degrade while nitrophenol is a very widely used pollutant. We will describe conditions and parameters that we have used and discuss the results that we have obtained to show the successful degradation of these important pollutants

120. Multifunctional Binary METAL Oxide Composite Nanostructures

Alex Ibhaden¹, Gilian Greenway² and Yue Yue, University of Hull, United Kingdom, (1)Faculty of Science and the Environment and Hull Environment Research Institute, University of Hull, Cottingham Road, Hull HU6 7RX, United Kingdom. (2)Department of Chemistry, University of Hull, Cottingham Road, United Kingdom HU6 7RX

Multifunctional catalysis and novel catalyst materials and composites are needed to achieve safer chemical processing, greener chemistry and future sustainability. One of the important properties required in these applications is the nanostructure of the composite materials. We report here the synthesis and characterization of binary oxide $\text{TiO}_2 - \text{RuO}_2 - \text{SiO}_2$ nanoparticles of defined particle characteristics and enhanced functionality. High temperature hydrogen reduction reactions enables the synthesis of binary metal oxide composite nanostructures based on titanium, ruthenium and silicon precursor materials. Surface characterization using XRD, SEM and raman spectroscopy was supplemented by BET measurements using Micromeritics analysis. Results indicate that the incorporation of silicon ions into the titania precursor materials resulted in increased surface area and enhanced catalytic activity. Charge transfer across the interface of the composite materials occurs when these materials are used as catalysts in oxidation reactions. This study also examined the growth morphology, thermal stability and geometric structure and how these affect the reactivity of these materials. The surfaces of these materials were also modified using a surface modifier and long chain surfactants and used for the decomposition of an industrial water pollutant, methyl orange. Results indicate that compared to commercially available materials, the surface modified composite materials were 15–20% more efficient as catalysts in these reactions.

121. Adsorption and Reaction of Multifunctional Oxygenates on Transition Metal Surfaces

J. Will Medlin, University of Colorado, Boulder, CO

To produce fuels and chemical products from biomass feedstocks, new processes capable of selective conversions of highly oxygenated compounds must be developed. The general biorefinery concept requires the production of a set of “building block” compounds from fermentation or chemical treatment of sugars, and the subsequent conversion of these compounds into a variety of value-added derivatives. A major challenge in the design of solid catalysts for these conversions of the relevant building blocks is that these oxygenated molecules contain multiple functional groups that may interact with the catalyst surface, causing problems in achieving selective conversion at a single position on the building block molecule. Related processes are of importance in the fine chemicals industry. We have investigated the adsorption and reaction of several model multifunctional oxygenates (including unsaturated oxygenates and polyols) on the (111) surface of Pd and Pt using a combination of surface spectroscopies and density functional theory calculations. This contribution will focus on the detailed surface reaction mechanisms observed on the two surfaces and on possible methods by which more selective catalysts may be designed for these applications.

122. Development of An Enzymatic Process for Lipitor

Michael P. Burns¹, David W. Bauer², Alastair Denholm³, Aoife Fahy³, Cathal Healy³, John O’Shaughnessy³, Éanna O’Maitiú³, Floriana Stomeo³, Gillian Whittaker³ and John W. Wong¹, (1)Pfizer, Groton, CT, (2)Pfizer, Kalamazoo, MI, (3)Pfizer, Cork, Ireland

A process for the biocatalytic reduction of (*R*)-*tert*-butyl 6-cyano-5-hydroxy-3-oxohexanoate was developed and implemented at commercial scale. The resulting (3*R*,5*R*)-*tert*-butyl 6-cyano-3,5-dihydroxyhexanoate is a key intermediate in the synthesis of atorvastatin (Lipitor). The benefits of the biocatalytic process include elimination of hazardous and toxic reagents, elimination of cryogenic reaction conditions and multiple distillations, reduction of organic solvent waste, and improved product purity and quality.

123. Biocatalytically Synthesized Polypyrrole

Ramaswamy Nagarajan¹, Rahul Garhwal¹, Subhalakshmi Nagarajan¹, Jayant Kumar¹, Ferdinando F. Bruno² and Lynne A. Samuelson², (1)University of Massachusetts Lowell, Lowell, MA, (2)U.S. Army RDECOM Natick Soldier Center, Natick, MA

Among electrically conducting polymers polypyrrole has attracted tremendous attention over the past decade due to the ease of synthesis and relatively lower toxicity. This suggests its wide range of potential applications especially in medical diagnostics. However, conventionally, polypyrrole is been synthesized either electrochemically or chemically using strong oxidants which are often toxic or incompatible with biological systems. More recently it has been shown that oxidative polymerization reactions can be catalyzed by plant peroxidases. Here we report the template-assisted oxidative polymerization of pyrrole using soybean peroxidase in an aqueous non-toxic solvent system. In this study poly (sodium 4-styrene sulfonate) PSS is used as the polyelectrolyte template that provides water-solubility to the polypyrrole synthesized. PSS also provides the counter-ion for doped conducting polymer. Spectroscopic characterization indicates the formation of an electrically conducting polymer. The polypyrrole that could also be doped and de-doped reversibly exhibits characteristic spectral features similar to those reported for chemically/electrochemically synthesized polymer. Detailed characterization of the polymer formed under various reaction conditions will also be presented. This enzymatic route provides the opportunity to synthesize polypyrrole at a higher pH than reported earlier. The favorable pH combined with aqueous reaction media

supports the possibility of extending the use of polypyrrole to applications such as biomedical devices or biosensing where there may be a requirement to synthesize polypyrrole in the presence of the biological entity.

124. Biocatalytic Production of Unnatural Cyclic Secondary Amino Acids for Peptidomimetic Pharmaceuticals

John Grate, Codexis, Inc., Redwood City, CA

Unnatural cyclic secondary amino acids such as substituted proline and pipercolic acid derivatives appear in a number of peptidomimetic drug candidates in development. Examples include the unnatural 3,4-*cis*-fused bicyclic *L*-proline analogs that are key constituents in the peptidomimetic Hepatitis C virus protease inhibitors boceprevir (Schering-Plough, Phase 2) and telaprevir (Vertex, Phase 3). These are candidates for a first-in-class Hepatitis C therapy to address an important unmet medical need.

Prior chemical routes to produce these proline analogs are “steppy” and involve wasteful late separations of stereoisomeric mixtures. Codexis envisioned shorter processes that avoid separating stereoisomers involving biocatalytic desymmetrization of the corresponding 3,4-*cis*-fused bicyclic pyrrolidines (the starting materials for prior routes) to the single imine stereoisomer that is precursor to the *L*-amino acid.

Wild-type monoamine oxidases were identified that are capable of desired stereoselective oxidation of the symmetric cyclic amines to the desired asymmetric cyclic imines, but their characteristics were otherwise wholly inadequate to enable practical processes. They were poorly produced recombinantly and their catalytic activities and in-process stability are extremely poor. Applying its advanced directed evolution technologies, Codexis evolved monoamine oxidases that are readily manufactured and fit to enable the development of practical, scalable reactions. The subsequent steps provide the desired *L*-amino acids without any resort to separating stereoisomers. Process development also involved addressing some interesting reaction engineering issues, which will also be presented. These processes are now being scaled up to provide material for clinical trials.

126. Asymmetric Aldol Reaction Between Benzaldehyde and 2-Butanone in Coordinated Ionic Liquids

Dishun Zhao¹, Hongyan Cui¹, Erhong Duan² and Qian Li¹, (1)Hebei University of Science and Technology, Shijiazhuang, China, (2)Tianjin University, Tianjin, China

In recent years, ionic liquids have been extensively used in many organic synthesis reactions as potential green alternative solvents and catalysts. The asymmetric aldol reaction is one of the most efficient processes for the synthesis of optically active α -hydroxy carbonyl compounds which are important intermediates. The asymmetric aldol reaction have been extensively used to prepare pharmaceutical, pesticide, and flavor chemicals, have high yields and stereoselectivity and have good application foreground. Coordinated ionic liquids are new compounds on the basis of traditional ionic liquids, which have the same general nature as traditional ionic liquids, such as negligible vapor pressure, nonflammability, high thermal stability, electric chemistry window way big and wide liquid temperature range. Coordinated ionic liquids have a number of advantages over traditional ionic liquids including simple synthesis methods, short respond time, cheap raw material and atom-economy. In this study, four kinds of coordinated ionic liquids were synthesized using caprolactam and salts, which were confirmed by IR and NMR. In coordinated ionic liquids, direct asymmetric aldol addition of benzaldehyde and 2-butanone was investigated using *L*-proline as a chiral catalyst. The influences of various reaction parameters such as reaction time, respond temperature, cycle times, different coordinated ionic liquids and different molar ratios were discussed. The product was easily isolated and the coordinated

Abstracts, Continued

ionic liquid could be reused at least 4 times with almost the same efficiency. Using this method, the asymmetric aldol reaction was not only simplified but also a potential green alternative over traditional method.

127. Natural Capitalism

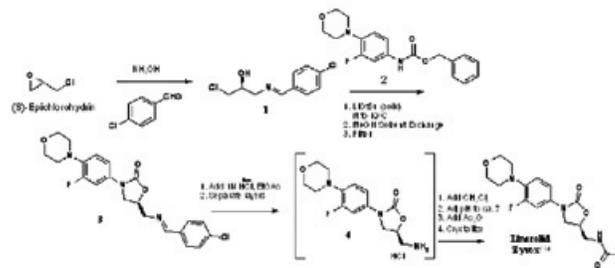
Stuart A. Jones, Interface Americas, Inc., LaGrange, GA

As an innovator of modular carpet, Interface is recognized as one of the leaders in industrial ecology. Having been on the sustainability journey for 13 years, Interface has a mature perspective of the challenges involved in reaching a sustainable future as both a company and a society. This sustainability focus is the differentiator for Interface in both its marketplace and the industrial market at large. Over the last 5 years, the core business has over doubled through sustainable innovation. The concept of Biomimicry and Life Cycle Analysis with practical examples of how the concepts are being used in the ideation and evaluation phases of the innovation process will be explored. Looking at the concept of environmental health as a leading indicator of business health vs. a trend in consumer awareness will give a perspective for those asking the question: "What is the business reason for going green?" Leadership and how vision galvanizes the activity of a business and instills purpose in the organization and culture of the associates and stakeholders will be explored. An introduction to the concept of Biomimicry, with a story of how a disruptive innovation came through the innovation process and ultimately launched into the market place will be discussed. The unique "Out of the Box Process" will be described. Also discussed will be Interface's development of a way to evaluate almost any decision on the premise of environmental health in a visual way that simplifies all of the complexities of the Life Cycle Analysis. This measurement system coupled with the traditional measure of economic return and social wellness combine to form a complete and balanced scorecard for the corporation.

128. Convergent Green Synthesis of Linezolid (Zyvox)

William R. Perrault, James B. Keeler, William C. Snyder, Christian L. Clark, Michael R. Reeder, Richard J. Imbordino, Rebecca M. Anderson, Nabil Ghazal, Stephen L. Seacrest and Bruce A. Pearlman, Pfizer, Kalamazoo, MI

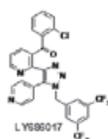
Pfizer has developed a novel, convergent, green, second generation synthesis of Linezolid (the active ingredient in Zyvox™). The second generation process will replace the launch process after approval by appropriate regulatory agencies and has numerous green chemistry benefits: overall yield is increased by 8%; total waste is reduced by 56%; non-recycled waste is eliminated. At current volumes, total waste will be reduced 1.9 million kilograms per year and 1.7 million kg per year non-recyclable waste will be eliminated. The improved process utilizes a highly efficient low dilution convergent synthesis to replace the more dilute linear synthesis utilized in the launch process. The key chlorohydrin imine reagent 1 contains both the chiral center and the key 5-*S*-aminomethyl moiety of linezolid. In the launch process, *S*-1-chloro-2,3-propanediol was utilized to install the oxazolidinone functionality. However, this yielded a 5-*S*-hydroxymethyl group which required activation as the 3-nitrobenzenesulfonate and displacement with excess ammonia to generate the corresponding aminomethyl group of linezolid. The second generation process affords the oxazolidinone imine 3 in the convergent step. The penultimate 5-*S*-aminomethyl oxazolidinone 4 is then easily formed via hydrolysis with stoichiometric hydrochloric acid. Acylation of this amine with acetic anhydride, utilizing an improved Schotten Baumann reaction, affords high purity linezolid.



129. A Practical and Green Chemical Approach for the Manufacture of NK1 Antagonist LY686017

Michael E. Kopach, Tony Zhang, Scott Coffey, Alfio Borghese, Michael Kobierski and William Trankle, Eli Lilly and Company, Indianapolis, IN

An innovative and environmental friendly route for the commercial production of an investigational new drug candidate LY686017, an antagonist of the Neurokinin 1 (NK1) subtype of tachykinin receptor, is described. LY686017 has undergone phase 2 clinical trials for the treatment of anxiety and irritable bowel syndrome (IBS). The improved route of manufacture delivers LY686017 in exceptionally high purity (>99.9%), a significant accomplishment considering the potential for positional isomers for all 5 aromatic rings. Eli Lilly and Company uses a metric called "e-factor" internally that is similar, but not identical to Sheldon's E factor. Lilly's e-factor is the total mass of all raw materials, including water that are used to produce each kg of active pharmaceutical ingredient "API" beginning from routinely available commercial starting materials. Despite the structural complexity of the API, the new route has a net e-factor of 146 kg/kg API, an 84% reduction relative to the original route executed for Phase I clinical trials. The selected commercial route for LY686017 was demonstrated on a pilot plant scale during 2006 in Indianapolis, Indiana. Two prior synthetic routes have been executed at pilot plant scale at Eli Lilly's Indianapolis, Indiana and Mount Saint Guibert, Belgium facilities, respectively. Improvement of key green chemistry parameters across the evolution of these route demonstrates the power of technical innovations and is testimonial to the importance of incorporating the 12 green chemistry principles to the design and definition of synthetic processes.



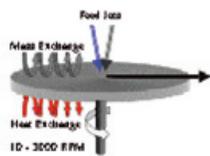
130. Synthesis of Amino Functionalised 2,4,6-Triarylpyridines and 1,5-Diketones Via Process Intensification on Rotating Surfaces

Nicole M. Smith, Marck Norret and Colin L. Raston, University of Western Australia, Crawley, Australia

Since Krohnke's original report on the synthesis of 2,4,6-triarylpyridines, there has been a plethora of research targeting their syntheses.¹ Nevertheless there are no reported simple 'one-pot' procedures for the synthesis of amino functionalized compounds, for example, 4'-aryl-2,6-bis(4-aminophenyl)pyridines. We have deemed these compounds as precursors for further elaboration en route to the synthesis of DNA binding ligands, in particular targeting G-quadruplex DNA which has recently received much attention as a possible target in cancer therapy.² We recently reported the efficient 'one-

pot' synthesis of 4'-(pyridyl)-terpyridines in polyethylene glycol (PEG)³ and the 'one-pot' synthesis of 4'-aryl-2,6-bis(4-aminophenyl)pyridines and their corresponding 1,5-diketone intermediates in PEG with high yield, purity and negligible waste.⁴ This 'one-pot' base catalyzed approach in making amino-substituted pyridines of this type is without precedent. Process intensification is another tool for green chemistry.⁵ It has been developed in the present study to prepare the intermediate 1,5-diketones in a single pass on a spinning disc processor (SDP) (Fig 1). This is associated with a residence time of ca 0.5 secs, whereas some reactions using traditional batch technology take several hours to go to completion.

Fig 1 Spinning Disc Processor (SDP) References: (1)Cave, G.W.V., Raston, C.L., J. Chem. Soc., Perkin Trans 1., 2001, 1, 3258; Cave, G.W.V., Raston, C.L., Chem. Commun., 2000, 2199; Rothenberg, G, Downie, A.P., Raston, C.L., Scott, J.L., J. Am. Chem. Soc., 2001, 123, 8701. (2)Waller, Z.A.E., Shirude, P.S., Rodriguez, R., Balasubramanian, S., Chem. Commun., 2008. (3)Smith, C.B., Raston, C.L., Sobolev, A.N., Green Chem., 2005, 7, 650. (4)Smith, M.N., Raston, C.L., Smith, C.B., Sobolev, A.N., Green Chem., 2007, 9, 1185. (5)Anantachoke, N, Makha, M, Raston, C.L., Reutrakul, V, Smith, N.C., J. Am. Chem. Soc., 2006, 128, 13847–13853.



131. The Synthesis of the Hollow Titanium Silicate Zeolite(HTS) and Its Application in Catalysis

Min Lin, Bin Zhu, Xingtian Shu and Xieqing Wang, Research institute of Petroleum processing, SINOPEC, Beijing, China

The titanium silicate zeolite(TS-1) shows a remarkable high efficiency and molecular selectivity in oxidation reactions under mild conditions. The selective oxidation of organic substrates by H₂O₂ in the presence of TS-1 is an interesting area of high potentiality for the development of new environmentally friendly technologies. The TS-1 synthesis, as a variety of useful oxidation reactions material, is a key process. Now, a hollow titanium silicate zeolite (HTS) has been commercial synthesized. The synthesized HTS sample was investigated by X-ray diffraction patterns, ²⁹Si MAS NMR spectra, FT-IR and N₂ adsorption. While the HTS was applied to oxidate the phenol into diphenol, the revulsive period has been shorten to one half. They has the 96~99% conversion in oxidation of cyclohexanone to oxim and the 95~98% conversion in oxidation of propylene to propylene epoxide. Now, the outstanding catalytic activity and selectivity of the HTS have made it a commercial catalyst for the manufacture of catechol and hydroquinone from phenol and the cyclohexanone ammoximation processes on industrial scale in China.

132. Solvent and Copper Free Sonogashira Reactions Utilizing High-Speed Ball Milling

Dennis A. Fulmer, University of Cincinnati, Cincinnati, OH

The technique of high-speed ball milling (HSBM) has recently been shown to provide a useful solvent-free route to the reduction of esters using a mild reducing agent. HSBM is a technique that utilizes a ball-bearing agitated at high speed to provide the energy for the reaction. Due to the noted differences in reactivity between HSBM and solution based chemistry, an investigation of coupling reactions was undertaken to produce a greener syntheses of these types of reactions.

Transition-metal-catalyst cross-coupling reactions are very important in the field of organic synthesis. Among these, the coupling between aryl halides and terminal alkynes to produce aryl alkynes, known as the Sonogashira reaction, is important for the manufacture of natural products, pharmaceuticals, and other organic materials. Traditionally, this reaction is carried out using a phosphane-palladium complex catalyst, catalytic copper halide, and triethyl amine. Among the several drawbacks in the use of Sonogashira couplings are high loadings of palladium catalyst and the use of copper salts. The presence of copper salt can promote homo-coupling of the reactants, thus resulting in

costly separation procedures and loss of valuable starting materials. A method that could result in the elimination of copper salts and solvents, while utilizing a low catalyst load would be desirable.

To date a method has been developed for a solvent-free Sonogashira coupling using HSBM conditions. Using this method it has been found that the use of copper salts is unnecessary. Also, it has been found that small catalytic loading is possible. Initial results indicate that the use of Pd(0) in place of a Pd(II) catalyst is possible. This represents a solvent and copper free methodology that results in the generation of less chemical waste, in a more atom economical manner.

133. A Collaborative Partnership to Develop Strategies for Waste Minimization and Solvent Recovery for the Celecoxib Process

Mariano J. Savelski¹, C. Stewart Slater¹, Gregory Hounsell², Daniel Pilipauskas² and Frank Urbanski², (1)Rowan University, Glassboro, NJ, (2)Pfizer, Inc., New York, NY

Through the engineering clinic program, Rowan University and Pfizer have collaborated to explore green engineering alternatives for waste minimization and solvent recovery for the celecoxib process. The current manufacturing process at the Barceloneta, Puerto Rico plant is being evaluated and several green engineering retrofit options proposed. The group has performed a design case study on isopropanol recovery from waste streams with extractive-distillation and pervaporation-distillation techniques. The case study describes equipment and processing issues, and estimates environmental impacts and costs. This project is one of several being conducted by Rowan University as part of the EPA Pollution Prevention initiative in the pharmaceutical industry.

134. Palladium Removal from Reaction Mixtures by Fixed Bed Adsorption

Michael J. Girgis¹, Laura E. Kuczynski², Sonia M. Berberena², Caitlin A. Boyd², Pamela L. Kubinski², Megerle L. Scherholz², Donald Drinkwater¹, Min Yang¹, Xiaoxuan Shen¹, Stan Babiak¹, Stephanie Farrell², Robert Hesketh² and Brian G. Lefebvre², (1)Novartis Pharmaceuticals Corporation, East Hanover, NJ, (2)Rowan University, Glassboro, NJ

The objective of this project, which was sponsored by Novartis Pharmaceuticals Corporation, was to remove palladium from a reaction mixture using a fixed bed adsorption column. Palladium is a heavy metal that is used frequently as a catalyst in many reactions in the pharmaceutical industry. Reaction mixtures can be contaminated up to 3000 ppm with palladium. A final drug substance can only contain two ppm palladium or less. For this project, the Heck coupling reaction of 4-bromobenzaldehyde and methyl acrylate was used, as it is representative of common reactions used in the pharmaceutical industry.

Adsorbents were evaluated by generating adsorption isotherms; Quadrapure TU was chosen as the adsorbent based on the high capacity of this resin at 60°C. The adsorption column is packed with Quadrapure TU resin and glass beads. Palladium concentration is determined using a novel HPLC method that is still in development, and verified through outside analytical lab analysis. Several adsorption column runs at various flow rates and packing geometries have been performed, with the overall goal of operating the column under conditions that promote full utilization of the resin bed. The effect of feed concentration, flow rate, and packing geometry will be discussed.

Abstracts, Continued

135. Process Improvement of a Crystallization Using a Green Engineering Approach

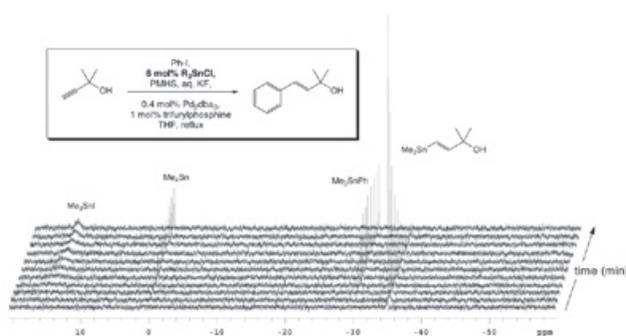
Daniel Sujo N.¹, Stephanie Farrell² and Robert P. Hesketh², (1)Siegfried (USA), Inc., Pennsville, NJ, (2)Rowan University, Glassboro, NJ

An industrial crystallization system was analyzed using a green engineering approach. The current method to crystallize a metal catalyst species is to using a stirred tank with a semibatch feed system. A double-feed reactor configuration was also examined and found to improve this process. This new scheme reduces the turnaround batch time by 90% and the environmental impact by 30%, compared to the current single-feed operation scheme. The experiments showed that operating in a double feed mode allowed the crystallization to be conducted at a constant pH which resulted in a high purity, larger particle size. From this, a high settling velocity was achieved and resulted in a reduction in batch time. In addition, additional experiments showed a relationship between the pH and the size of the agglomerates and the purity of the crystals. Further research on the crystallization mechanism and kinetics is strongly recommended.

136. Developments toward a Green Stille Reaction

Nicole M. Torres¹, William P. Gallagher² and Robert E. Maleczka Jr.¹, (1)Michigan State University, East Lansing, MI, (2)Bristol-Myers Squibb Company, New Brunswick, NJ

For over 30 years the Pd mediated cross-coupling of organostannanes with suitable electrophiles (aka the Stille reaction) has been utilized for the construction of sp²-sp² carbon-carbon bonds. Its continued popularity is in part due to high functional group tolerance, ease of synthetic access to organotin coupling partners, and the ability to control and retain the regio- and stereochemical outcome. Unfortunately, the toxicity of the organotin reagents and tin by-products makes this reaction environmentally unattractive. To alleviate the problems associated with organotin toxicity, including tin handling and dealing with stoichiometric amounts of tin waste, our group developed a one-pot hydrostannylation/Stille sequence that is catalytic in tin. Although the process was rendered catalytic, turnover numbers remain modest. Our attempts to improve these turnover numbers have been hampered by a lack of mechanistic understanding of the full role played by the organotin. To gain such insight, we are using ¹¹⁹Sn NMR to monitor the reaction kinetics and elucidate the pathways of the tin species. Recent results and their significance regarding the development of a green Stille reaction will be discussed.



137. Environmentally Attractive Metal-Catalyzed Reduction of Alkyl Halides

Jian Yang and Maurice Brookhart, UNC-Chapel Hill, Chapel Hill, NC

Reduction of alkyl halides to alkanes is a frequently practiced synthetic transformation. The most common method employed is the use of Bu₃SnH via a radical chain mechanism. Alternative reduction procedures are desired owing

to the toxicity of the tin reagents and problems separating tin byproducts from the desired organic products. We have discovered and developed a highly efficient and environmental friendly procedure for the reduction of primary, secondary and tertiary chlorides, bromides and iodides as well as certain fluorides by the cheap and readily available triethylsilane reagents with cationic iridium pincer catalysts. Dichloromethane is also rapidly reduced to methane.

In addition, catalyst loadings as low as 0.03% have proved successful and this process can be carried out in a solvent-free manner, which may provide an environmentally attractive and safe alternative to currently practiced reductions of alkyl halides. The scope and efficiency of the catalytic reaction, mechanistic details, and optimized experimental protocols will be presented.

138. The Greening of the Aerobic Oxidation of *p*-Xylene to Terephthalic Acid

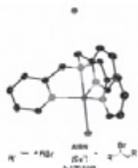
Walt Partenheimer, Consultant, DuPont (retired), Portland, OR

The invention of selective homogeneous catalysts in the last 60 years have led to the large scale manufacture of terephthalic acid, the major component of polyethylene terephthalate (PET). It will be shown how the greenness of these processes has increased first with the invention of the soluble cobalt compounds in acetic acid, then with the invention of the metal/bromide catalysts. It is the increase in the selectivity of these catalysts which are directly responsible for large reductions in the production of green-house gases (CO₂, CO, CH₃Br) and other rate decreasing and color producing by-products. The reduction in by-products and higher yields has also resulted in simplification of the purification of the terephthalic acid and of the commercial plants. The latest efforts to further enhance this greenness is through the invention of catalysts which can successfully oxidize *p*-xylene to terephthalic acid in high yield in 'hot' and supercritical water. The structure of MnBr₂, is the most successful catalyst in 'hot' water, has been determined. The structure of these homogeneous catalysts, their relationship to solvent properties, and their catalytic mechanisms which are responsible for the greatly enhanced selectivity are given.

140. Highly Efficient Copper Mediated Atom Transfer Radical Addition (ATRA) in the Presence of Reducing Agents

Tomislav Pintauer, Duquesne University, Pittsburgh, PA

Synthesis, characterization and exceptional activity of Cu^I(TPMA)Br (TPMA = tris(2-pyridylmethyl) amine) and [Cu^{II}(TPMA)Br][Br] complexes in ATRA reactions of polybrominated compounds to alkenes in the presence of reducing agent (AIBN) was reported. [Cu^{II}(TPMA)Br][Br], in conjunction with AIBN, effectively catalyzed ATRA reactions of CBr₄ and CHBr₃ to alkenes with concentrations between 5 and 100 ppm, which is the lowest number achieved in copper mediated ATRA. The molecular structure of Cu^I(TPMA)Br indicated that the complex was pseudo pentacoordinated in the solid state due to the coordination of TPMA (Cu^I-N = 2.1024(15), 2.0753(15), 2.0709(15) and 2.4397(14)) and bromide anion to the copper(I) center (Cu^I-Br = 2.5088(3)). Variable temperature ¹H NMR and cyclic voltammetry studies confirmed the equilibrium between Cu^I(TPMA)Br and [Cu^{II}(TPMA)(CH₃CN)][Br], indicating some degree of halide anion dissociation in solution. The coordination of bromide anion to [Cu^I(TPMA)]⁺ cation resulted in a formation of much more reducing Cu^I(TPMA)Br complex (*E*_{1/2} = -720 mV vs. Fc/Fc⁺) than the corresponding ClO₄⁻ (*E*_{1/2} = -422 mV vs. Fc/Fc⁺) and PF₆⁻ (*E*_{1/2} = -421 mV vs. Fc/Fc⁺) analogues. In [Cu^{II}(TPMA)Br][Br], the Cu^{II} atom was coordinated by four nitrogen atoms (Cu^{II}-N_{eq} = 2.073(2) and Cu^{II}-N_{ax} = 2.040(3)) from TPMA ligand and a bromine atom (Cu^{II}-Br = 2.3836(6)). The overall geometry of the complex was distorted trigonal bipyramidal. Cu^I(TPMA)Br and [Cu^{II}(TPMA)Br][Br] complexes showed similar structural features from the point of view of TPMA coordination. The only more pronounced difference in the TPMA coordination to the copper center was observed in the shortening of Cu-N_{ax} bond length by approximately 0.400 on going from Cu^I(TPMA)Br to [Cu^{II}(TPMA)Br][Br].



141. Novel Metal Oxide Catalysts and Process for Methacrylic Acid Production Using Isobutane as the Feedstock

Manhua Mandy Lin, EverNu Technology LLC, Maple Glen, PA and Krishnan Pillai, EverNu Technology LLC, North Brunswick, NJ

Methacrylic acid (MAA) and its methyl ester methyl methacrylate (MMA) are high-volume commodity chemicals serving as building blocks for various polymers widely used in construction, automobile, appliances and coating industries. The 2005 US MAA/MMA production was ~1.8 billion pounds. Since 1930s, MAA/MMA has been produced in the US using the conventional Acetone Cyanohydrin (ACH) process, which requires acetone and hydrogen cyanide (HCN) as the feedstocks. The production of 1 ton of MAA requires at least 0.31 ton HCN. The ACH process further requires using a large quantity of concentrated H₂SO₄ as solvent and catalyst. The production of each ton of MAA further requires using 1.6 tons of concentrated H₂SO₄, while generates 1.2 tons of ammonium bisulfate requiring disposal. In 2005 alone, the US production of 1.82 billion pounds of MAA/MMA a) consumed 558+ million pounds of HCN, b) used/regenerated ~2.88 billion pounds of concentrated H₂SO₄; c) generated/dispensed ~2.16 billion pounds of ammonium bisulfate.

EverNu has developed a patent-pending catalyst and process which uses isobutane (and air) as the feedstock for the production of MAA. Using isobutane as the feedstock has three major benefits. It offers significant economical benefit since isobutane cost is only a fraction of that of acetone and HCN. It further offers tens of trillion Btu of energy benefit per year, since isobutane partial oxidation is isothermic and the need to recycle H₂SO₄ is eliminated. The environmental benefit is enormous and it includes: a) completely eliminating the use of large quantities of HCN and H₂SO₄, b) avoiding the generation/disposal of the toxic/corrosive wastes relating to the use of HCN and H₂SO₄; and c) use of non-toxic feedstock isobutane is inherently much safer with regards to workers' exposure and accident potential. Further, isobutane can be obtained from renewable sources in the future, as indicated by some recent research.

142. Catalytic Reforming of *n*-Heptane on Platinum-Zinc Supported on Gamma-Alumina

Mehdi Vadi, Islamic Azad University Fasa Branch, Fasa, Iran and Hamid Daneshvar, Islamic Azad University Firozabad Branch, Firozabad, Iran

The series of mono-metallic and bi-metallic catalysts have been prepared by impregnating with solutions containing compound of H₂PtCl₅·Zn(NO₃)₂ and 1ml HCl (0.1 mol). The activity and selectivity of the catalysts have been determined under conditions at 450–5000°C 15–30atm. Molar ratio H₂/C₇H₁₆=5 and WH=1.5/h for converting *n*-heptane. Under these experimental conditions it has been established that the conversion of *n*-heptane into branched aliphatic isomers is catalyzed by a bifunctional mechanism. The results show that when Zn is present, the catalysts are much more stable and have much higher selectivities for aromatization reaction. At a given conversion the bimetallic catalysts produce much higher concentrations of cracked products. It is shown that Zn modifies the acidity of the support, resulting to higher selectivity for aromatization and lower selectivity for cracking and also modifies the properties of the Pt.

143. Catalytic Reforming of *n*-Heptane on Platinum-Copper Supported on Gamma-Alumina

Mehdi Vadi, Islamic Azad University Fasa Branch, Fasa, Iran and M. Mozafare, Islamic Azad University Firozabad Branch, Firozabad, Iran

The series of mono-metallic and bi-metallic catalysts have been prepared by impregnating with solutions containing compound of H₂PtCl₅·Cu(NO₃)₂ and 1ml HCl (0.1 mol). The activity and selectivity of the catalysts have been determined under conditions at 450–5000°C 15–30atm. Molar ratio H₂/C₇H₁₆=5 and WH=1.5/h for converting *n*-heptane. Under these experimental conditions it has been established that the conversion of *n*-heptane into branched aliphatic isomers is catalyzed by a bifunctional mechanism. The results show that when Cu is present, the catalysts are much more stable and have much higher selectivities for aromatization reaction. At a given conversion the bimetallic catalysts produce much lower concentrations of cracked products. It is shown that Cu modifies the acidity of the support, resulting to higher selectivity for aromatization and lower selectivity for cracking and also modifies the properties of the Pt.

144. Catalytic Reforming of *n*-Heptane on Platinum-Rhenium Supported on Gamma-Alumina

Marjan Bazargane, Islamic Azad University Firozabad Branch, Firozabad, Iran and Mehdi Vadi, Islamic Azad University Fasa Branch, Fasa, Iran

The series of mono-metallic and bi-metallic catalysts have been prepared by impregnating with solutions containing compound of H₂PtCl₅·Re(NO₃)₃ and 1ml HCl (0.1 mol). The activity and selectivity of the catalysts have been determined under conditions at 450–5000°C 15–30atm. Molar ratio H₂/C₇H₁₆=5 and WH=1.5/h for converting *n*-heptane. Under these experimental conditions it has been established that the conversion of *n*-heptane into branched aliphatic isomers is catalyzed by a bifunctional mechanism. The results show that when Nb is present, the catalysts are much more stable and have much higher selectivities for isomerization reaction. At a given conversion the bimetallic catalysts produce much lower concentrations of cracked products. It is shown that Re modifies the acidity of the support, resulting to higher selectivity for isomerization and lower selectivity for cracking and also modifies the properties of the Pt.

145. Ecomate—Environmentally Benign Foam Blowing Agent

John A. Murphy and John F. Timberlake, Foam Supplies Inc, Earth City, MO

Insulation foams are a critical component in the effort to reduce the amount of energy expended for heating and cooling, thus reducing CO₂ emissions and our dependence on foreign oil. The critical component of these foams is the captured cell gas, and its insulative capability. These gases have formerly been CFCs, HCFCs, and now HFCs which, despite their many virtues, have been shown to contribute to global warming and ozone depletion.

Ecomate® [methyl formate] is an environmentally sound alternative foam insulation blowing agent. It is non-Ozone Depleting [zero ODP], has little to no Global Warming Potential [GWP], and has such a minimal effect on photochemical smog production that the USEPA has declared it to be VOC exempt. Ecomate is the only foam blowing agent on the market with these superior credentials.

For every ton of ecomate used in replacement of HFC blowing agent, there is a savings of over two thousand tons of CO₂ equivalents [GWP]. And since ecomate does not contribute to photochemical smog, it can be used in Air Pollution Containment Districts without disrupting the environment, nor displacing jobs.

Abstracts, *Continued*

While the transition from CFCs, to HCFCs, to HFCs has meant compromised thermal efficiencies in the foams produced by each succeeding transition, it has been shown that ecomate can produce foams with equivalent thermal properties to those obtained with current HFCs.

Since ecomate requires only half as much material as current HFCs to achieve an equivalent density, it becomes even more environmentally benign, not to mention more cost effective. Using ecomate instead of HFCs will dramatically reduce the long term emission of Greenhouse Gases from polyurethane insulating foams without additional environmental impact.

146. Future Designs of Pressure Sensitive Adhesives

Steven J. Severtson, University of Minnesota, Saint Paul, MN, Carl Houtman, USDA, Forest Products Laboratory, Madison, WI and Larry Gwin, Franklin International, Columbus, OH

Over the past ten years there has been considerable progress in the development of pressure sensitive (PS) products such as labels, stamps and notes that are recycling compatible. These are paper products containing pressure-sensitive adhesive (PSA) that can be incorporated into post-consumer waste without interfering with the paper recycling process. The most promising designs appear to be those that limit the fragmentation of PSA films during the processing of secondary fiber. This results in residual PSA particles that are removed with high efficiency from the process with conventional mill contaminant control equipment. The modifications required to achieve these environmentally friendly designs are relatively minor and can be accomplished by adhesive producers and converters without raising costs or sacrificing performance. In this presentation, our research, development and commercialization efforts on recycling compatible PS products are reviewed. Results for both hot-melt and water-based acrylic PSA will be summarized as well as the roles additives and laminate design play in determining the impact of adhesive films on recycling operations. Characteristics of recycling compatible PS laminates will be outlined as well as methods for incorporating these into products while maintaining performance properties. Also discussed will be future trends in PS products and our progress in identifying structural requirements for compostability.

147. Powder Coatings Based on Seed Oils

Jim D. Earls, Fabio Aguirre, Maurice J. Marks and Jerry E. White, The Dow Chemical Company, Freeport, TX

The Dow Chemical Company has a number of active development projects on going for seed oils and their derivatives in industrial applications. In the work reported in this paper, multi-functional acid derivatives from castor oil and reductively hydroformylated soy bean oil methyl esters were evaluated in hybrid powder coating systems. In comparison to incumbent polyester-epoxy materials used in these applications, the findings to date for the seed oil modified systems indicate the following advantages: 1) control of gloss can be obtained and desired matte-like finishes produced, 2) faster cures at lower temperatures which may provide utility in coating heat sensitive substrates, such as wood, 3) lower viscosities which would provide improved substrate wet out and 4) improved scratch resistance, a desirable property for many applications. In addition to these performance improvements lower costs for hybrid powder systems may be ultimately possible for the global powder coatings market of which hybrid systems account for 50% of the materials used.

148. Photo Polymer Systems for Environmentally Benign Preparation of Films and Coatings

Emily Stoler and John C. Warner, Warner Babcock Institute for Green Chemistry, Woburn, MA

The addition of photochemically active moieties to a polymer structure allows materials to be made that can undergo post-synthesis reactions. Because the photoactive materials are embedded covalently to the polymers, there is no leaching of reagents in the final products. Aqueous coating systems have been designed to undergo various phototransformations that affects properties including solubility, strength and polymer/surface compatibility. This technology presents an environmentally benign method for the preparation of numerous industrially relevant films, masks and coatings.

149. Synthesis and Properties of a New Seed Oil-Based Thermoplastic

Jerry E. White, Jim D. Earls, John W. Sherman, Leonardo C. Lopez and Marvin L. Dettloff, The Dow Chemical Company, Freeport, TX

Oxidation of undecylenic acid, a derivative of castor oil, affords 10,11-epoxyundecanoic acid which in the presence of phosphonium halide can undergo an A-B step-growth polymerization via nucleophilic ring opening of the epoxy group by the carboxylic acid moiety to yield a semi-crystalline ($T_m = 97^\circ\text{C}$), hydroxy-functionalized aliphatic polyester. This new thermoplastic exhibits yield stress, break stress and elongation (9.7 MPa, 24.1 MPa and 450%) similar to those of low density polyethylene. However, in contrast to the behavior of the polyolefin and owing to the pendent hydroxy moieties populating the polymer backbone, films of the polyester adhere strongly to metallic substrates and have moderately good barrier to oxygen. In addition to a detailed discussion of the physical and thermal properties of the polyester, the mechanism of the formation and consequent molecular weight distribution of this new polymer will be described.

150. New Value-Added Materials from Ethanol by-Products

George E. Inglett, S. Kim, J. Xu, D. Stevenson, D. Chen and S. Liu, USDA-ARS-NCAUR, Peoria, IL

Value-added materials were obtained from a distiller's dried grains (DDG) sample obtained from MCP Corporation. It was processed by jet cooking at various pH levels and fractionated. Among the various fractions, free flowing particles were obtained that appear to have several opportunities for a range of industrial applications. Rheological properties were measured by several techniques including RVA pasting values. Some of the compositional and chemical aspects of the new materials were measured. Their moisture, ash, protein, and oil contents were determined. Also evaluations of their antioxidant properties of the various materials were made and some of the fractions were found to be considerably elevated.

151. Integrating Green Engineering Concepts Across Disciplines

Sean P. McGinnis, Virginia Tech, Blacksburg, VA

Approaches for integrating green engineering concepts across engineering disciplines will be discussed based on the experiences of the Green Engineering Program at Virginia Tech. This program was initiated over a decade ago with a broad mission in education, outreach, and research. In some respects this program might be considered an example of best-practices, while in other respects it is a case study for the challenges of interdisciplinary education.

The educational core of this program is an 18-credit green engineering concentration which has recently been approved as a minor. This curriculum is flexible from a student perspective due to an extensive list of approved courses

from a variety of departments. The fact that nearly all of the courses exist independent of the green engineering program facilitates the interdisciplinary scope of such a program in an otherwise rigid department-focused institutional structure. However, there are both recurring issues and long term concerns that will be discussed for a program which stands independent and separate from departments.

Recently, efforts have been made to expand the interdisciplinary nature of the program beyond an extensive menu of courses crossing engineering disciplines. An NSF-sponsored interdisciplinary senior design project which incorporates concepts of green engineering and sustainability as well as formally researches engineering education methods is in a pilot phase. Exposure of green engineering concepts to liberal arts students has also occurred by collaborating with a unique 2-year curriculum in which a cohort of undergraduate students receives broad university credits by considering the theme "Earth Sustainability" across disciplines in their freshman and sophomore years. Consideration of these new efforts as well as the approaches of other institutions to incorporate green engineering concepts provides a diverse and growing number of opportunities which potentially offer significant improvements in the impacts of green engineering education.

152. Making It Easier to Be Green—a Green Online Curriculum Free to the World

Terrence Collins and Chip Walter, Carnegie Mellon University, Pittsburgh, PA
It's not easy being green, especially in the field of chemistry. But it's important. For the most part, the traditional approach to teaching synthetic chemistry has been to train students to become very good at combining molecules in elegant and creative ways without much thought about the damage their creations might do. At Carnegie Mellon University, we are transforming the green chemistry courses we have been teaching for fifteen years into interactive, online coursework, which will be made available world-wide, and free of charge. This will create a virtual, online "place," where scientists, teachers, students and researchers everywhere can gather and learn about green chemistry and related sustainability challenges. It will also enable these thinkers to interactively share their insights, and speed the dissemination of their hard work, as it pools a global well-spring of intellectual capital and encourages debate and discussion. Our hope? A new generation of green chemists capable of designing a sustainable civilization at the level where the world is truly built—the molecular level.



153. Beyond Green Engineering: Fostering the Ethic That Powers the Action

Linda Vanasupa¹, William Hughes² and Trevor Harding², (1)California Polytechnic State University, San Luis Obispo, CA, (2)California Polytechnic State University, 93407, CA

One of the approaches to green engineering is to teach the tools that enable engineers to make design decisions that are better for the environment. While knowing these tools is necessary, recent studies of graduates indicate that it may not be sufficient; graduating engineers lag other college graduates in some measure of cognitive development that underpin the green engineering ethic. The implication is that curricula must be altered to simultaneously build the ability to use the tools and build the needed ethic. In our program, we have been able to integrate five major elements within our curriculum to foster this ethic. These elements were derived from a holistic model of student development and closely align with the framework advanced by Peter Senge in his book, "The Fifth Discipline." The elements include: shared vision, personal mastery, team learning, reflecting on mental models, and systems thinking. In this paper, we present examples of how these elements are utilized in the curriculum as well as data showing accelerated development of students' moral development and ability to function on design teams.

154. Learning Materials and Teaching Strategies for Sustainability Integration in Engineering Education

Qiong Zhang¹, Julie Zimmerman², James R. Mihelcic¹ and Linda Vanasupa³, (1) Michigan Technological University, Houghton, MI, (2)Yale University, New Haven, CT, (3)California Polytechnic State University, San Luis Obispo, CA

As the world faces increasing threats to the long-term health of the environment, society, and economy, sustainability has emerged and now is gathering the attention of undergraduate and graduate education across many campuses in the U.S. To integrate sustainability into engineering education, effective learning materials and teaching strategies have to be created that enables engineering faculty to more easily incorporate sustainability approaches into curricula.

In this paper, new learning materials will be introduced including an innovative textbook titled Environmental Engineering: Fundamentals, Sustainability, Design and one example of in-course modules Introduction to Sustainability. The intended audience for the new textbook is undergraduate civil and environmental engineering (CEE) students and the textbook introduces sustainability into the discussion of fundamentals in CEE. In-course modules are designed to be readily integrated into existing science and engineering courses and can be used by faculty beyond CEE to introduce sustainability into their fundamentals discussions. The identical interdisciplinary engineering courses "Green Engineering and Sustainability" to be implemented at both Michigan Tech and Yale University will be introduced and educational innovations in the form of student-to-student networks will be discussed.

The concept of incorporating and leveraging Fink's taxonomy of significant learning in the design of the textbook, the module and the green engineering courses will be introduced and discussed. The paper will also introduce the assessment approach designed to measure students' progress within several dimensions of Fink's taxonomy, including Learning how to learn (self-directed learning), Foundational knowledge (understanding of the connections between engineering solutions and global issues), Application (ability to design for sustainability), Caring (motivation, interest), and Human dimension (moral reasoning). The end of the paper will discuss how the textbook and the teaching/learning practices employed in the green engineering courses align with principles for good practice in undergraduate education and demonstrated successful teaching methods in engineering education.

Abstracts, *Continued*

155. Building the Capacity of Green Chemistry Educators

Julie Haack and James E. Hutchison, University of Oregon, Eugene, OR

Over the past decade considerable progress has been made toward developing a foundation for green chemistry education. Collaborative efforts by the American Chemical Society Green Chemistry Institute, the Environmental Protection Agency and the National Science Foundation in partnership with national leaders in green chemistry education have facilitated the incorporation of green chemistry principles into the curriculum by removing two significant barriers to adoption; (1) educating faculty and students about green chemistry principles (via summer workshops and symposia at national meetings) and (2) increasing the availability of educational materials that can be incorporated into the curriculum (GEMs database <http://greenchem.uoregon.edu/gems.html>). As a result, we see a growing number of community college and university faculty who have adopted the curriculum and are now interested in contributing to the development of new educational materials. One approach to increasing access to these materials is to invest in building the capacity of educators to sustain the development of innovative "green" education materials. This presentation will describe the development, delivery and assessment of a capacity building workshop for green chemistry educators that was held in Washington, D.C. in June 2007. Based on post-workshop surveys and interviews, we observed a significant increase in the capacity of participants to contribute to the development and dissemination of new green chemistry materials. We will also discuss important lessons learned and describe some of the unanticipated benefits and challenges of capacity building in this community.

156. Students Game to Learn about Green Supply Chains

Jacqueline A. Isaacs, Northeastern University, Boston, MA

The desire to address complex technological and social issues in an engaged manner inspired the development of a prototype board game created to raise the awareness of environmental issues in engineering. Over the past decade, both massively multiplayer games and simulation games have reached new levels of sophistication and retained enormous mainstream audiences. Developments in digital technology allow new opportunities to engage students in collaborative and active learning. Designed for in-class play by undergraduate and graduate engineering students as well as business students, the computer game is based on team competition of companies in the automobile supply chain, with the objectives set to achieve the highest profit and lowest environmental detriment.

The game is played using stakeholders in the manufacturing supply chain in the automotive industry. Six students create a team of three suppliers: materials, parts, and cars. Within this team, two students take on roles for each of the three companies in the supply chain. Within the ten rounds in the game, each company within the supply chain takes its turn to invest and select among different technologies in three areas for each company: production, storage and waste disposal. There are tradeoffs in investment costs and green values for each technology option, and there is a hierarchy to the innovation options available for each turn. The students work within their team and budget to try to create the most profitable and green supply chain. Successful game strategy requires both cooperation and competition for players to succeed.

Students learn facts along multiple dimensions, including: the history of environmentally benign technologies over the past decades; environmental policies and legislation that influence manufacturing in the global economy; current business strategies and technologies used in industry to address environmental burdens; tradeoffs among economic and environmental policies that influence technology; and team-based decision-making.

157. Connecting Industry to K-12 Education through Green Chemistry

Rachel Pokrandt, Beyond Benign, Woburn, MA

Strategies and success stories around creating partnerships and initiatives between business and K-12 school communities will be discussed in this presentation. Local school communities including students, teachers, administrators and parents can be wonderful avenues to increase the reach of an industrial green chemistry initiative. Strategies and resources will be discussed and shared with a view to getting industry personnel out into school communities to share green chemistry initiatives and connect with the green chemistry leaders of the future.

158. Gas Phase Conversion of Sugar/Sugar Alcohol to Valuable C3 Chemicals

Wei Yan, Ali Tekeci, Joshua M. Ronco and Galen J. Suppes, University of Missouri-Columbia, Columbia, MO

Conversion of sugar/sugar alcohol to value-added chemicals had been widely studied. Especially for higher sugars, research has been widely exclusively on liquid phase reactions with much emphasis on catalytic hydrogenolysis. The hydrogenolysis reactions are performed at high hydrogen pressure to achieve high conversion and selectivity. In this paper, gas phase catalytic hydrogenolysis is evaluated as a means to overcome liquid phase hydrogenolysis barriers associated with high pressures and catalyst deactivation. Copper-chromite, palladium, and nickel pellet catalysts were screened in gas phase hydrogenation and dehydration of sorbitol and glucose. Complete conversions were attained at reaction pressures of 0.3 to 1bars. The highest selectivities were to acetol.

160. Improved Immobilization of Chiral Bisoxazolines on Silica: Application to Circulating Flow-Type Pack Bed Reactor

SuSeong Lee, Jaehong Lim and Jackie Y. Ying, Institute of Bioengineering and Nanotechnology, Singapore, Singapore

Spherical siliceous mesocellular foam (MCF) was synthesized by simple modification of the conventional method and partially surface-modified with trimethylsilyl (TMS) groups prior to the immobilization of chiral bisoxazoline (box). Following the ligand immobilization, the support was postcapped with TMS groups by vapor-phase grafting. This two-step modification of siliceous MCF support led to superior catalyst enantioselectivity. The resulting MCF-immobilized box-Cu(I) catalyst provided 95% ee for trans isomer and 92% ee for cis isomer, and 80% yield for the asymmetric cyclopropanation of styrene. It was also successfully recycled 12 times without losing any enantioselectivity and reactivity. The partial TMS precapping of MCF represents an effective means of preparing a suitable silica support for immobilizing a wide variety of chiral box ligands and nitrogen-containing ligands. This approach can be applied to achieve well-dispersed chiral ligands without strong interactions with the silica surface, so that excellent enantioselectivity, reactivity and recyclability can be attained.

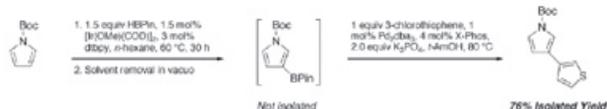
It is also found that flexibility of linker group, precapping, catalyst loading amount, and postcapping are very important factors to be duly considered to get an excellent heterogeneous catalyst in the case of immobilization of chiral azabox. The optimal MCF-supported azabox-Cu(I) catalyst offered as high enantioselectivity and yield as the homogeneous counterpart, and excellent recyclability. This study demonstrated that silica-supported catalysts could achieve comparable enantioselectivity and yield as their homogeneous counterparts through proper design. In addition, the heterogenized catalyst with the optimal ligand loading density could attain superior chemoselectivity in a short reaction time with increased productivity. The optimal heterogenized catalyst was successfully applied to a circulating flow-type packed bed

reactor, while retaining the attractive enantioselectivity, yield and recyclability. The circulating flow-type reactor was more suitable than the conventional continuous flow reactor for gas-generating processes, such as the cyclopropanation reaction.

161. Catalytic Borylation for Efficient Elaboration of Aromatic Compounds

Ghayoor A. Chotana, Venkata A. Kallepalli, Anna M. Norberg, Luis A. Sanchez, Britt A. Vanchura, Robert E. Maleczka Jr. and Milton R. Smith III, Michigan State University, East Lansing, MI

Organoboron species are useful building blocks for pharmaceuticals and other valuable materials because B–C bonds can be manipulated almost at will. For example, the Suzuki–Miyaura coupling of boronic acids or esters with alkenyl or aryl halides and their triflates is a mild, and versatile method that has revolutionized the construction aryl C–C bonds. While alkyl boron reagents are commonly obtained by hydroboration of olefins, aryl boronic acids and esters are usually prepared from the corresponding aryl halide. The thermal, catalytic coupling of C–H and B–H bonds that was invented in 1999 has emerged as an efficient method for preparing boronic acids. It is attractive because the Ir catalysts typically employed are functional group tolerant (alkyl, halo-, carboxy, alkoxy-, and protected amino), regioselective, and efficient. The direct production of aryl and heteroaryl boronic esters from hydrocarbon feed stocks with hydrogen gas as the sole byproduct minimizes waste streams and reduces the energy requirements associated with aryl boronate synthesis. Moreover, the borylation products can often be transformed *without* isolation. Recent advances and applications of this chemistry will be presented.



162. Decarboxylative Coupling of Aromatic Carboxylic Acids with Aryl Iodides and Unfunctionalized Arenes

Adelina M. Voutchkova, Abigail Coplin and Robert Crabtree, Yale University, New Haven, CT

The use of carboxylic acids as partners in transition metal catalyzed biaryl coupling reactions is increasingly being explored, but the few reported reactions suffer from harsh reaction conditions and limited substrate scope. We report a microwave-assisted unsymmetric coupling in which readily available carboxylic acids are decarboxylated and coupled to either aryl halides or unfunctionalized arenes via C–H activation to give biaryl products in good to excellent yields. The catalyst system consists of a homogeneous palladium complex which catalyzes the cross coupling reaction, as well as a silver or copper salt which aids the decarboxylation of the aromatic carboxylate. Microwave heating enhances the yield, reduces the reaction time to 2–5 minutes and affords cleaner reactions than conventional methods.

164. Phase Behavior and Rheological Analysis of Cellulose Nanocrystal Aqueous Suspensions

Esteban E. Ureña-Benavides and Christopher L. Kitchens, Clemson University, Clemson, SC

Cellulose nanocrystals (CNCs) have potential to become a renewable and cost effective alternative for biocompatible polymer nanocomposites with a high strength to weight ratio. However, these particles are usually very polydispersed and non-compatible with hydrophobic polymers. Aqueous suspensions of rod shaped CNC were prepared by sulfuric acid hydrolysis of ashless cellulose

powder and kraft pulp from a local paper mill. The particles are less than 10 nm wide, and 20 to 300 nm long. The chiral nematic—isotropic phase behavior of aqueous CNC suspensions has been investigated by measuring the relative volume, concentration and particle size as a function of cellulose concentration, and temperature. Successive partition of both phases has been used to partially fractionate the particles by size into more uniform distributions with average lengths of 125 nm, 154 nm, and 207 nm. Transmission Electron Microscopy was used to measure the nanocrystals obtained from the isotropic and anisotropic phases to determine the effects of nanocrystal size on the phase behavior and degree of fractionation. Rheological analyses have been used to characterize the fluid behavior of the nanocrystal suspensions as a function of cellulose concentration, particle size, and nanocrystal ordering. This provides a fundamental understanding of the interactions between the particles and the media in which they are dispersed. We are currently investigating the aqueous surface modification via esterification, and etherification of the nanocrystal's hydroxyl groups to make the particles hydrophobic. Nanocomposites filled with CNC have usually shown little improvement on their properties, presumably because of the poor compatibility with the polymeric matrix. The surface modification, as well as, size fractionation of the particles are intended to improve the dispersability and compatibility of the cellulose crystals within biodegradable and biocompatible polymers; leading to a new generation of green materials.

165. “Green” and Size-Controlled Synthesis and Seed-Mediated Growth of Pd Nanoparticles

Juncheng Liu and Christopher B. Roberts, Auburn University, Auburn, AL

Central to the concept of seed-mediated growth of nanoparticles is that small nanoparticle seeds serve as nucleation centers to precisely grow nanoparticles to a desired size. Herein we present an environmentally benign and size-controlled seed-mediated growth method coupled with an organic phase extraction to yield monodisperse dodecanethiol capped Pd nanoparticles. Monodisperse Pd nanoparticles (ca. 3.4 nm, standard deviation: 0.6 nm) were first synthesized and stabilized by a “green” and inexpensive polysugar, sodium carboxymethyl cellulose (CMC) in aqueous solution. The monodisperse Pd nanoparticles were subsequently employed as seeds on the surface of which fresh Pd²⁺ ions were reduced by weak reducing agent ascorbic acid. We optimized the processing conditions that favor controlled growth on the nanoparticle seeds versus formation of new nucleation sites, thereby yielding improved control over particle size with narrow size distribution. Using different amount of salt in this seed-mediated growth process, different sized Pd nanoparticles were controllably synthesized. Finally, the nanoparticles were extracted from aqueous solution into an organic phase by using dodecanethiol as extractant with the assistance of HCl. The advantage of the seed-mediated growth method used in this study is that the Pd nanoparticle size could be precisely controlled (from 3.4 to 7.6 nm) by simply varying the ratio of the seed to Pd salt added in the growth stage. Furthermore, the use of environmentally friendly reagents, such as water (solvent), CMC (capping agent) and ascorbic acid (reducing agent) in the system provides both “green” and cost-effective merits for this precise size-controlled particle synthesis method.

166. Synthesis of Nanophase Mn(VII) Oxide Using Green Technology and Its Applications

R. K. Vempati, Southern Methodist University, Dallas, TX, Gajanan Bhat, University of Tennessee at Knoxville, Knoxville, TN and Richard Wagner, Phycology, Inc., Indianapolis, IN

The innovation focuses on the formation and stabilization of innovative nanophase Mn(VII) oxide (NM7O) using 1,4-phenylenediamine (PDA). The starting material is a beige-colored hydrated Mn(II) mineral which upon addition of PDA forms a violet-colored NM7O. The mechanisms of formation appear to be oxidation of PDA to 1,4-benzoquinone in the presence of air

Abstracts, *Continued*

resulting in oxidation of the hydrated Mn(II) mineral to NM70. The SEM analysis showed globular NM70 mass with particle size ranging from 50 to 100 nm, and cyclic voltammetry and optical spectroscopy confirmed the Mn7+ oxidation state. Based on laboratory studies, NM70 is a super Lewis acid in that it attacks compounds with lone pairs of electrons, e.g. cyclohexylamine and cyclohexanone. Additionally, neutralize chemical warfare agents (CWAs) surrogates, e.g., 2-chloroethyl ethylsulfide (CEES-mustard gas analog) and dimethyl methylphosphonate (DMMP-sarin gas analog). The applications developed are: 1) odor removal from N and S bearing compounds, 2) metal polish, 3) disulfide syntheses using thiol groups, and 4) algacide and bactericide formulations. Also, the violet-colored NM70 after reduction changes to environmentally safe brown-colored Mn(IV) oxide, and this property can be exploited to develop an optical sensor. The NM70 has been successfully coated/impregnated into non-woven and melt blown fabrics. These fabric materials can be incorporated into clothing, wipes and liners for odor control, algae and bacterial growth control and destruction, metal polish, toxic spills, decontamination, and diapers, hospital beds, incontinence, undergarments for soldiers and astronauts for odor removal and prevent bacterial growth. The NM70 manufacturing technology has received a US patent, a patent is pending on chemical warfare agents' destruction, and two provisional patents filed on NM70 coated fabrics and destruction of nuisance and pathogenic microorganisms. Green technologies relating to domestic, industrial, healthcare, hygiene and military and homeland security applications are being developed.

167. Expanding the Horizons of Green Battery and Capacitor Chemistries with Nano-Porous Carbon

Bryan D. Sawyer and Galen Suppes, University of Missouri-Columbia, Columbia, MO

Energy storage is an empowering technology for many power technologies that are more sustainable and green (e.g. wind and solar power). Also, batteries and capacitors allow green energy alternatives to be used in electric (BEV, HEV, and PHEV) vehicles as one of the most promising alternatives to gasoline. One of the most benign, high-performance materials in batteries and capacitors is nano-porous carbon.

This paper is on the use of ALLCRAFT nano-porous carbon in supercapacitors. At surface areas in excess of 3,400 m²/g, the ALLCRAFT carbon has about 50% more surface area than the best reported material used in supercapacitors. Performance in several supercapacitor configurations will be reported.

168. Novel Green Chemistries to Extend Automobile Catalytic Converter Useful Life While Reducing Exhaust Gaseous Emissions

Ewa Bardasz, The Lubrizol Corporation, Wickliffe, OH

For the last 50 years, phosphorus in the form of zinc dialkyldithiophosphate (ZDDP) has been the most cost-effective antiwear, antioxidant and anticorrosion component of engine oil. When ZDDP fulfills its function in the engine, the phosphorus can enter the exhaust stream, either by consumption or volatilization (released as a vapor). This phosphorus interacts with and decreases the effectiveness of catalytic converters used by automotive manufacturers to reduce exhaust gas emissions. This phenomenon, called catalyst deactivation, inhibits auto manufacturers' ability to meet United States Environmental Protection Agency requirements for a 120,000-mile or 10-year catalyst system warranty.

In 1994, the United States engine oil industry set a limit for the amount of phosphorus engine oil could contain. The maximum of 0.08wt% phosphorus continues to be the limit today. Although a phosphorus limit was set to protect catalysts, the phosphorus present in the oil still can volatilize from the engine and react with the catalyst to cause catalyst deactivation. It is known that some ZDDPs are more prone than others to volatilize and therefore deactivate catalysts.

Concerns about losses in catalyst efficiency forced formulators either to design engine oils with lower concentrations of traditional ZDDP or to develop cost-effective, low-volatility ZDDP technology. In 2004, The Lubrizol Corporation introduced its patent-pending, low-volatility ZDDP technology to provide engine oil formulators with an alternative to designing higher-cost engine oils with lower levels of ZDDP.

169. Polymer-Filled Composite Membranes

Xiangwu Zhang, North Carolina State University, Raleigh, NC

Proton exchange membrane fuel cells (PEMFCs) are promising candidates for "clean" power generation because they provide electricity without combustion and pollutants associated with burning fossil fuels. Perfluorosulfonic acid polymer membranes, such as Nafion[®], are typically used as the electrolyte in low-temperature PEMFCs because of their excellent chemical, mechanical, and thermal stability, as well as their relatively high proton conductivity of ca. 0.08 S cm⁻¹. However, the proton transport requires continuous water assistance, and as a result, Nafion[®] membranes have limited operating temperature (< 100°C) because of the dehydration at high temperatures. Increase in membrane operating temperature can lead to high-temperature PEMFC technology, which solves or avoids many shortcomings associated with low-temperature PEMFC technology, including slow electrode kinetics, low CO tolerance, and difficult heat dissipation.

In this work, polymer-filled porous silica composite electrolyte membranes [porous silica-polystyrenesulfonic acid (porous silica-PSS)] were introduced by attaching polystyrenesulfonic acid (PSS) onto the inner surface of porous silica. The proton conductivity of porous silica-PSS increases with increase in surface proton density, and the highest conductivity (0.05 S cm⁻¹ at 150°C) is obtained at a surface proton density of 15.2 nm⁻². It is also found that there is no dramatic conductivity drop for porous silica-PSS membranes at temperatures higher than 100°C, indicating that a high operating temperature has been achieved.

Cell potentials of porous silica-PSS-based fuel cell and Nafion[®] 115-based fuel cell were measured. At 65°C, Nafion[®]-based fuel cell has higher cell potential than porous silica-PSS-based fuel cell. However, when the temperature increases to 130°C, the cell potential of Nafion[®]-based fuel cell drops dramatically because of the low operating temperature of Nafion[®] membrane. Porous silica-PSS-based fuel cell has even higher cell performance at 130°C than at room temperature, which may be caused by improved electrode reaction kinetics at elevated temperature.

170. Providing Real-Life Experience While Learning Green Chemistry Principles

Dalila G. Kovacs, Grand Valley State University, Allendale, MI

The challenges brought up by population, energy, global changes, resource depletion, food supplies, and environment pollution impose fundamental changes in the education of the 21st century work force. Teaching elements of industrial chemistry should follow a new approach starting from this challenges imposed by the status of the global economy, world affairs, and the future of humankind. Naturally for an academic institution the solution is to introduce students to Green Chemistry principles and their application in industrial processes early in their careers. For this purpose, at Grand Valley State University we design a new undergraduate course, Green Chemistry and Industrial Processes. However, a better solution is to use the class as a vehicle to provide our students not only with theory and philosophical principles but also with the opportunity to manifest their creativity in applying the green chemistry principles to existing, unsolved problems in industrial scaled processes. To achieve this goal, we are working to establish a committed partnership among the local area businesses interested in 'greening' their production and/or operation and our students. The business is to provide a real-life problem, while the students will aim toward new and innovative

approaches to solve it. The principles and classic cases of Green Chemistry would serve as a base for the students to inquire and discover, while being encouraged to be creative. In the process, the student will gain knowledge and understanding of industrial processes based on green chemistry principle. They will take responsibility for solving real-life problems, by investigating and reflecting on the application of 'green' processes currently in-use and propose creative solutions to the problem they engaged in solving. The business will gain exposure to the local student population and opportunity to present the business successes while they actively participate in the education of West Michigan's future workforce.

171. Towards the Greening of Our Minds: A New Course Offered at Washington College, Chestertown, MD

Anne E. Marteel-Parrish, Washington College, Chestertown, MD

Environmentally friendly scientists are increasingly conscious about the need to make chemistry "greener". A new course titled "Towards the Greening of Our Minds: Green and Sustainable Chemistry" was developed at Washington College, Chestertown, MD. The goal of this course is to present a different perspective regarding chemistry and its applications in academia and industry worldwide. This course covers both the theoretical and practical aspects of green and sustainable chemistry.

The presentation will focus specifically on the content of the course which is divided in the following five sections:

- The first section provides the foundations of green chemistry and sustainability.
- The second section focuses on some of the applications of green chemistry and sustainability in academia and industry.
- The third section is allotted to the writing of a four-page article about one of the annual Presidential Green Chemistry Challenge Awards and to the oral presentation of the accomplishments of the award recipient.
- The fourth section addresses the status of green chemistry and sustainability in developing countries followed by a discussion about the book by William McDonough and Michael Braungart entitled "Remaking the Way We Make Things: Cradle to Cradle".
- The fifth section is based on the presentation of a team mini-proposal. A team of students needs to apply their greener mind to a chemical reaction, process or product that is not environmentally friendly and come up with an alternative design.

Taking this course, the students have the opportunity:

- To enrich existing knowledge about general and organic chemistry while learning about green chemistry and sustainability concepts,
- To critically evaluate policy decisions using green chemistry as the focus,
- To polish scientific writing and oral presentation skills,
- To develop leadership aptitude in discussions, and
- To build up confidence.

172. Teaching Students about Consumer Exposure to Hazardous Chemicals

Shonali Laha, Florida International University, Miami, FL

The requirement of one introductory environmental engineering class has now become mandatory in most undergraduate programs in Civil Engineering. We have such a class (ENV 3001) offered at Florida International University. Since the consensus ranking of environmental problem areas on the basis of population cancer risks (U.S. EPA, 1987) lists indoor air quality, pesticide residues on foods, and consumer exposure to chemicals among the top four areas of concern, I have attempted to introduce an understanding of risk assessment and the control of such risks through personal choices in every day

matters. In one assignment I require my students to list the household products that they use to control for pests like cockroaches and ants, and then they need to examine the active chemical ingredients of these products including their toxicity, environmental persistence, etc. We discuss the general evolution of pesticide science over the past century and the nature of the health hazards individuals expose themselves to. We also talk about less harmful alternatives that might work to control pests. Since indoor air quality has become an increasingly significant concern as U.S. residents spend most of their lives in indoor environments, we also argue about the merits of turning off the air conditioning systems at home and allowing our houses/apartments to be well aired for at least six months in a year. This offers the added advantage of reducing our greenhouse gas emissions or our carbon footprint. In addition to these more personal choices, the introductory environmental engineering class offers a review of mass and energy concepts, environmental chemistry, looks at water and air quality issues, as well as teaches students about basic municipal water and wastewater treatment, air pollution control and solid and hazardous waste treatment.

173. Using the Rowan University Engineering Clinic Model to Implement Green Engineering Partnerships with the Pharmaceutical Industry

C. Stewart Slater, Mariano J. Savelski, Brian G. Lefebvre, Stephanie Farrell and Robert P. Hesketh, Rowan University, Glassboro, NJ

Rowan University Engineering Clinic projects have examined how to apply green engineering strategies to both R&D and manufacturing. This has been accomplished through industry-university partnerships with pharmaceutical companies (Bristol-Myers Squibb, Novartis, Pfizer) in the New Jersey area. Several grants from the U.S. Environmental Protection Agency and industry have supported initiatives in green chemistry, engineering and design in our Engineering Clinic program. The green engineering clinic projects use a junior/senior student team who work with the industrial partner on approaches to pollution prevention. Students are able to learn about green engineering design and apply their knowledge directly to a real industrial case through faculty and industrial mentoring. These projects have the potential to yield green engineering outcomes such as: process intensification, waste reduction, and energy reduction. The Rowan Clinic model allows companies in the region to take advantage of university expertise to assist in sustainable development and manufacturing.

174. Understanding and Implementing the Principles of Green Chemistry in Industry

Amy S. Cannon, Beyond Benign: A Warner Babcock Foundation, Woburn, MA

Industrial leaders today are focused on promoting sustainability in their businesses. From energy usage in the work environment to recycling, sustainable practices are becoming standard. While these "operations" efforts are extremely important, chemical and manufacturing companies also have an opportunity to integrate sustainability into their fundamental technologies through green chemistry. Perhaps one of the most effective ways of ensuring a sustainable future is through the implementation of the principles of green chemistry at the research and development bench. This presentation will discuss techniques for teaching the principles of green chemistry to the industrial chemist and methods to implement the learned practices in an industrial setting.

Abstracts, *Continued*

175. C2B2—a Biorefining Collaboratory

John R. Dorgan¹, Alan Weimer², Ryan T. Gill², Will Medlin², Kenneth F. Reardon³ and Al Darzins⁴, (1)Colorado School of Mines, Golden, CO, (2) University of Colorado at Boulder, Boulder, CO, (3)Colorado State University, Fort Collins, CO, (4)National Renewable Energy Laboratory, Golden, CO

The Colorado Center for Biofuels and Biorefining (C2B2) is a research consortia combining three universities, a National Laboratory, the State Government, and a host of industrial sponsors. Under the auspices of the Colorado Renewable Energy Collaboratory, the Colorado School of Mines, Colorado State University, and the University of Colorado at Boulder are working with the Department of Energy's National Renewable Energy Laboratory (NREL) to advance the science and engineering of biorefining. C2B2 is also providing training and education necessary for meeting the workforce demands of new "Green Collar" jobs. The consortia brings together global energy, chemical, and agricultural companies to address the issues relevant to providing renewable based fuels and materials. Here, an overview of C2B2's research and educational activities is presented with an emphasis on new developments in thermochemical conversions, algae derived biodiesels, biorefining separations, and bioproducts (fuels and plastics).

176. 2008 BREEN FELLOWSHIP RECIPIENT: Biocatalytic Approaches to the Asymmetric Oxidation of Sulfides and Alkenes

Antonio Osorio-Lozada and Horacio F. Olivo, The University of Iowa, Iowa City, IA

Oxidation reactions are considered one of the transformations causing the most environmental footprint. Our group is interested in developing green processes to carry out oxidative transformations incorporating biocatalysts. We are interested in developing microbial and chemo-enzymatic processes that are attractive to the chemical and pharmaceutical industries. Asymmetric oxidations are of particular interest in developing chiral molecules for enantioselective syntheses.

Modafinil is a unique CNS stimulant that lacks any addiction liability. We developed a very short enantioselective route to one of its enantiomers. This new route employs microorganisms containing oxidative enzymes capable to deliver a desired sulfoxide in a highly enantioselective manner. Currently, modafinil is being investigated for the treatment of cocaine and metamphetamine addicts, and in the treatment of ADHD.

Our group is also currently developing an asymmetric chemo-enzymatic oxidation of alkenes. Epoxidation of indene is of particular interest to our group. Indene oxide is a valuable starting material for the syntheses of indinavir (Merck's HIV protease inhibitor), several chiral catalysts (Jacobsen's Cr(III) Schiff base), and also for the synthesis of a new chiral auxiliary developed in our group. Having a green asymmetric epoxidation process of indene will be attractive to the chemical and pharmaceutical industries. We will present two successful applications of green chemistry principles in the efficient preparation of useful compounds for synthetic and medicinal chemists.

177. 2008 HANCOCK AWARD RECIPIENT: Utilization of Linear-Dendritic Copolymers as Aqueous Nano-Reactors for Greener Cycloaddition, Oxidation and Polymerization Syntheses

Arsen Simonyan¹ and Ivan Gitsov², (1)State University of New York, Syracuse, NY, (2)Institute for Polymer Research, Syracuse, NY

The general scope of this study is the development of a supramolecular device that can be modified to serve as an efficient nano-scale reactor for organic reactions operating at green conditions. The reactions investigated have gradually become a key to a number of important materials for both the fine synthesis and the multi-ton scale industry thus emphasizing an increasing need

for cheap, high yield and environmentally friendly synthetic procedures. Our first strategy employs previously synthesized linear-dendritic block copolymers, based on benzyl-ether dendrons and poly(ethylene oxide), as the sole building blocks of self-assembled well-defined nano-reactors for model aqueous Diels-Alder and [4+4]-addition reactions that involve the practically water-insoluble reactants: fullerene[60], anthracene and naphthalene. The second approach involves the construction of nano-containers with embedded biocatalyst. The same linear-dendritic copolymers are used to envelop the enzyme laccase and form a stable complex in water. This nano-construct enables aqueous oxidation and/or polymerization reactions of hydrophobic compounds like anthracene, fullerene[60], curcumin, bisphenol A, steroids, to name a few. The results obtained in both strategies show that significant improvement of the rates could be achieved, leading to generally higher yields in shorter times than previously reported, with no organic solvents required during the reactions. In addition, the results obtained at this time further substantiate the environmental benefits of the strategies used by overall lower energy consumption, usage of non-toxic, renewable and/or recyclable reaction media and catalysts, simple recovery of reaction products, and last but not least, potential for easy transfer of technology to other substrates and reactions.

178. KeLa Energy Clean Coal Technology

Larry Moot, KeLa Energy LLC, Orlando, FL

KeLa Energy, LLC has developed a coal based, synthetic fuel made up of coal fines, recycled binding materials, and biomass. This water resistant synthetic fuel burns cleaner than coal (lower SO_x and NO_x) and can be engineered to meet the needs of the customer in terms of emissions, Btu value, and biomass content. Combustion chemistry taking place during the burning of the KeLa Fuel acts to "self-scrub" and lower the air emissions when compared to coal. KeLa Engineered Fuel does not breakdown in the presence of water and can be transported, stored and handled like coal. KeLa Engineered Fuel reuses what is currently a by-product of coal production that is sent to massive landfills. This technology represents a green engineering application of a several valuable resources.

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