Type them into questions box!

“Why am I muted?”
Don’t worry. Everyone is muted except the presenter and host.
Thank you and enjoy the show.

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Research Associate
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Nanomaterial Design Guided by the Principles of Green Chemistry

Thursday, May 18 @ 2-3pm ET

How can green chemistry be applied to nanotechnology to achieve the high performance needed for advanced applications while preventing or reducing health and environmental impacts? Join James Hutchison from the University of Oregon as he discusses the foundations for greener nanotechnology and presents a case study that uses nanomaterial product innovation guided by green chemistry.

Register Now!

What You Will Learn

- The opportunity to achieve a net environmental benefit by bringing together green chemistry with nanoscience
- The role that green chemistry plays in designing high performance nanomaterials and efficient nanomaterial production
- How green chemistry and nanoscience can be used together to develop innovative new products with environmental benefits


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The division is dedicated to supporting the efforts of chemical manufacturers, industrial and academic researchers, and science teachers at all levels to work for a safe and healthful work environment. Through our technical symposia, the Division’s Journal, the Journal of Chemical Health and Safety, our workshops and our DCHAS-L listserv, we provide a forum for scholarly health and safety research, advice and counsel from an experienced group, and support for health and safety efforts in industry and academia.

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Jason Sello, Associate Professor of Chemistry, Brown University
Courtney Aldrich, Associate Professor, Department of Medicinal Chemistry, University of Minnesota and Editor-in-Chief of ACS Infectious Diseases

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Creating a 21st Century Chemical Research Laboratory:
*Hazard Assessments and Fundamentals*

Kendra Leathy Denlinger
Graduate Student, University of Cincinnati

Ralph Stuart,
Chemical Hygiene Officer, Keane State College and Secretary, ACS CH&S

Slides available now! Recordings are an exclusive ACS member benefit.

This ACS Webinar is co-produced by the ACS Division of Chemical Health and Safety and the ACS Green Chemistry Institute
CREATING A 21ST CENTURY CHEMICAL RESEARCH LABORATORY: HAZARD ASSESSMENTS AND FUNDAMENTALS

Dr. Kendra Leahy Denlinger
University of Cincinnati

Ralph Stuart, CIH, CCHO
Chemical Hygiene Officer, Keene State College
Secretary, Division of Chemical Health and Safety, American Chemical Society

MAY 11, 2017

SAFETY WITHIN THE ACS VISION

ACS Chemistry for Life® Strategic Plan for 2017 and beyond

Passion for Chemistry and the Global Chemistry Enterprise
Focus on Members
Professionalism, Safety, and Ethics
Diversity and Inclusion
Lab Safety involves both Technical and Cultural Skills

20th Century:
Selecting Controls Based on Rules, guided by Chemical Intuition

21st Century:
a Safety System based on documented Risk Assessment

TECHNICAL CHEMICAL SAFETY RESOURCES

High school

- NFPA 45 requirements for instructional and educational labs, 2015

Undergraduate teaching labs

- Safety in Academic Chemistry Laboratories, 8th edition, 2017

“Mentored” research labs


Research laboratories

- Prudent Practices, 2011
- Identifying and Evaluating Hazards in Research Laboratories, 2016
- PubChem Laboratory Chemical Safety Summaries, 2016
- Pistoia Chemical Safety Library, 2017
RESEARCH RISK ASSESSMENT RESOURCES

National Research Council, 2011

ACS
(at the behest of the CSB)

PDF Version 2013

Web Version, 2016

OTHER KEY TECHNICAL TOOLS

National Library of Medicine’s Pubchem

Laboratory Chemical Safety Summaries (2015)

• Safety information on 103,000 chemicals

• Includes SDS-style information as well as specific reaction information between chemicals

Pistoia Alliance Chemical Safety Library (2017)

• Information on specific lab scale chemical incidents

• Access is free upon registrantion and reporting of incidents is encouraged.
CULTURAL LAB SAFETY RESOURCES

High school

Undergraduate education labs
- Creating Safety Cultures in Academic Institutions from ACS, 2013
- Laboratory Safety Guidelines, ACS Committee on Professional Training, 2015

“Mentored” research labs
- A Guide to Implementing a Safety Culture in our Universities from the APLU, 2016
- ACS Safety Guidelines for the Chemistry Professional 2017

Research lab work
- Safe Science from the National Research Council, 2014
- ACS journals policy, 2016

KEY RESEARCH SAFETY CULTURE RESOURCES

National Research Council, 2014

ACS, 2016
Which hazard MOST concerns you?

• Chemicals of known reactivity
• Chemicals of known toxicity
• Environmentally hazardous chemicals
• Chemicals of unknown toxicity
A LESSON IN LAB SAFETY

Chemical formula for Benzene

**SH**

**LC₅₀ ≤ 2.0 mg/L**

**HAZARD ASSESSMENT**

Safety in the laboratory requires a full team effort to be successful. When everyone in the laboratory understands how to identify hazards, assess risk, and select the appropriate control measures to eliminate a hazard or minimize risk, accidents, injuries, and near misses can be reduced.

https://www.acs.org/hazardassessment
**HAZARD VS. RISK**

### Know the Difference Between a Hazard and a Risk

<table>
<thead>
<tr>
<th>Hazard</th>
<th>Risk</th>
</tr>
</thead>
<tbody>
<tr>
<td>A hazard causes harm.</td>
<td>Risk is the probability that a hazard will cause harm.</td>
</tr>
<tr>
<td>A hazard can be eliminated, but not reduced.</td>
<td>Risk associated with a hazard can be reduced.</td>
</tr>
</tbody>
</table>

Risk = hazard x exposure

---

HIGH-SPEED BALL MILLING

BALL MILLING VS. SOLUTION
CHROMATOGRAPHY

Table 5.8 Column Chromatography Materials

<table>
<thead>
<tr>
<th>Stationary Phase</th>
<th>Moving Phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alumina</td>
<td>Increasing water</td>
</tr>
<tr>
<td>Silicic acid</td>
<td>Increasing ethanol</td>
</tr>
<tr>
<td>Magnesium sulfate</td>
<td>Increasing methanol</td>
</tr>
<tr>
<td>Cellulose paper</td>
<td>Increasing acetone</td>
</tr>
<tr>
<td></td>
<td>Ethyl acetate</td>
</tr>
<tr>
<td></td>
<td>Diethyl ether</td>
</tr>
<tr>
<td></td>
<td>Methylene chloride</td>
</tr>
<tr>
<td></td>
<td>Cyclohexane</td>
</tr>
<tr>
<td></td>
<td>Pentane</td>
</tr>
</tbody>
</table>

Functionalized polymer resins

Polystyrene 1-2% Cross-linked with divinylbenzene


FUNCTIONALIZED POLYMER RESINS

Filter paper
Funnel

Choose a green solvent.

Polymer (and anything attached to it) remains in filter paper.

Solvent (and anything dissolved in it) ends up in round-bottomed flask.
Design the reaction so that:

- A **product** is attached to the polymer
- A **byproduct** is attached to the polymer
- A **catalyst** is attached to the polymer

![Polystyrene 1-2% Cross-linked with divinylbenzene](image)

**WITTIG REACTION**

- 1950’s
- Nobel Prize awarded in 1970’s
- Harmful organic solvents
- Very strong bases (n-BuLi)
Have you developed Green Chemistry alternatives for specific reactions in your lab work?

- Yes, we have developed a full set of GC alternatives
- Yes, we have developed some GC alternatives
- Yes, we have developed a few GC alternatives
- No, we have not developed any GC alternatives yet
DETERMINE THE SCOPE

Collect Appropriate Background Information

The analysis team will need appropriate background information, including:

- Equipment diagrams
- A list describing common hazards associated with chemicals and gases
- A list of the equipment's chemical and gas compositions, operating pressures, flow rates, run times, and other applicable parameters
- Potential health and physical hazards of equipment (e.g., ionizing or nonionizing radiation, high temperature, high voltage, or mechanical pinch points)
- Equipment safety features (e.g., interlocks)
- Physical access to equipment, as necessary/possible

Safety Data Sheets can include a lot of this information.

Assemble Your Team

Everyone should be involved in hazard assessment, regardless of experience level or title in the lab.

Everyone is responsible for familiarizing themselves with appropriate controls for the hazards discovered in the lab.

Everyone is responsible for participating in hazard analyses (checklists, Job Hazard Analysis, and What-if Analysis) and the updating of the lab's Standard Operating Procedures. This is also a good time to review accidents, incidents, and near misses and collectively brainstorm ways to prevent these events in the future.

More experienced members of the team should lead risk assessment activities and assign risk ratings to the materials and processes in your lab.

Learn about the roles and responsibilities of various people in the lab.
CONDUCTING A HAZARD ASSESSMENT

Identify hazards → Analyze risks → Select controls

Identify hazards → Analyze risks → Select controls

Ways to Conduct a Hazard Assessment

<table>
<thead>
<tr>
<th>Hazard Assessment</th>
<th>Fundamentals</th>
<th>Ways to Conduct Assessments</th>
</tr>
</thead>
<tbody>
<tr>
<td>What-if Analysis</td>
<td>Job Hazard Analysis</td>
<td>Checklists</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Standard Operating Procedures</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Control Banding</td>
</tr>
</tbody>
</table>

fundamentals of hazard assessment | scoping and assembling your team | ways to conduct hazard assessments | tools
Identify hazards → **Analyze risks** → Select controls

---

**Calculate Risks Using Probability of Occurrence and Severity of Consequences Scaling**

Many risk assessments use "probability of occurrence" and "severity of consequences" scales to rate risks associated with laboratory experiments. They are comprehensive assessment tools and provide greater differentiation of risks based on actual laboratory operations.

Using this kind of scaling, laboratory hazard risk rating is calculated as follows:

\[
\text{Risk Rating (RR)} = \text{Probability of Occurrence (OV)} \times \text{Severity of Consequences Value (CV)}
\]

As the formula indicates, the higher the assessed probability of occurrence and severity of consequences, the greater the risk rating will be.

---

### Probability of Occurrence with Standard Linear Scaling

<table>
<thead>
<tr>
<th>Occurrence Value (OV)</th>
<th>Probability of Occurrence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Not Present</td>
<td>0%</td>
</tr>
<tr>
<td>Rare</td>
<td>1-10%</td>
</tr>
<tr>
<td>Possible</td>
<td>10-50%</td>
</tr>
<tr>
<td>Likely</td>
<td>50-90%</td>
</tr>
<tr>
<td>Almost Certainties</td>
<td>90-100%</td>
</tr>
</tbody>
</table>

### Severity of Consequences, Weighted Value Scale

<table>
<thead>
<tr>
<th>Consequence Value (CV)</th>
<th>Impact to...</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Risk</td>
<td>None</td>
</tr>
<tr>
<td>Minor</td>
<td>Minor injuries, Moderate impact, Moderate delays, Moderate damage</td>
</tr>
<tr>
<td>Moderate</td>
<td>Moderate to life threatening injuries, Additional resources required, Significant delays, Substantial damage</td>
</tr>
<tr>
<td>High</td>
<td>Life threatening injuries from single exposure, Severe loss of confidence</td>
</tr>
</tbody>
</table>

- high probability x no consequences = 4
- low probability x life threatening consequences = 20
Identify hazards → Analyze risks → Select controls

Hierarchy of Controls

- Prevent the hazard
- Isolate people from the hazard
- Change the way people work
- Protect the worker with Personal Protective Equipment

Physically remove the hazard

Elimination

Substitution

Engineering Controls

Administrative Controls

PPE

Source: http://www.cdc.gov/niosh/topics/hierarchy
ELIMINATION AND SUBSTITUTION

The San Destin Declaration: 9 Principles of Green Engineering*

1. Engineer processes and products holistically, use systems analysis, and integrate environmental impact assessment tools.
2. Conserve and improve natural ecosystems while protecting human health and well-being.
3. Use life-cycle thinking in all engineering activities.
4. Ensure that all material and energy inputs and outputs are as inherently safe and benign as possible.
5. Minimize depletion of natural resources.
6. Strive to prevent waste.
7. Develop and apply engineering solutions, while being cognizant of local geography, aspirations, and cultures.
8. Create engineering solutions beyond current or dominant technologies; improve, innovate, and invent (technologies) to achieve sustainability.


Meeting was supported by EPA, NSF, DOE (Los Alamos National Lab), and the ACS GCI.

“How can we tell if what we’re doing is actually greener?”

Green Chemistry Metrics

How interested are you in a Green Chemistry metrics tool that incorporated job hazard assessment considerations?

- Very interested
- Somewhat Interested
- Neither interested or disinterested
- Somewhat disinterested
- Very disinterested
**WASTE MINIMIZATION**

![Chemical reaction diagram](image)

*Figure 1. Comparison of solution-based Wittig (top) against mechanochemical Wittig (bottom).*


---

**MEASURING WASTE MINIMIZATION – THE ECScale**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Penalty points</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Yield</td>
<td>((100 - % \text{yield})/2)</td>
</tr>
<tr>
<td>2. Price of reaction components (to obtain 10 mmol of end product)</td>
<td></td>
</tr>
<tr>
<td>Inexpensive (&lt; $10)</td>
<td>0</td>
</tr>
<tr>
<td>Expensive (&gt; $10 and &lt; $50)</td>
<td>3</td>
</tr>
<tr>
<td>Very expensive (&gt; $50)</td>
<td>5</td>
</tr>
<tr>
<td>3. Safety</td>
<td></td>
</tr>
<tr>
<td>N (dangerous for environment)</td>
<td>5</td>
</tr>
<tr>
<td>T (toxic)</td>
<td>5</td>
</tr>
<tr>
<td>F (highly flammable)</td>
<td>5</td>
</tr>
<tr>
<td>E (explosive)</td>
<td>10</td>
</tr>
<tr>
<td>F+ (extremely flammable)</td>
<td>10</td>
</tr>
<tr>
<td>T+ (extremely toxic)</td>
<td>10</td>
</tr>
<tr>
<td>4. Technical setup</td>
<td></td>
</tr>
<tr>
<td>Common setup</td>
<td>0</td>
</tr>
<tr>
<td>Instruments for controlled addition of chemicals</td>
<td>1</td>
</tr>
<tr>
<td>Unconventional activation technique</td>
<td>2</td>
</tr>
<tr>
<td>Pressure equipment, &gt; 1 atm</td>
<td>3</td>
</tr>
<tr>
<td>Any additional special glassware</td>
<td>1</td>
</tr>
<tr>
<td>(Inert) gas atmosphere</td>
<td>1</td>
</tr>
<tr>
<td>Glove box</td>
<td>3</td>
</tr>
<tr>
<td>5. Temperature/time</td>
<td></td>
</tr>
<tr>
<td>Room temperature, &lt; 1 h</td>
<td>0</td>
</tr>
<tr>
<td>Room temperature, &lt; 24 h</td>
<td>1</td>
</tr>
<tr>
<td>Heating, &lt; 1 h</td>
<td>2</td>
</tr>
<tr>
<td>Heating, &gt; 1 h</td>
<td>3</td>
</tr>
<tr>
<td>Cooling to 0°C</td>
<td>4</td>
</tr>
<tr>
<td>Cooling, &lt; 0°C</td>
<td>5</td>
</tr>
<tr>
<td>6. Workup and purification</td>
<td></td>
</tr>
<tr>
<td>None</td>
<td>0</td>
</tr>
<tr>
<td>Cooling to room temperature</td>
<td>0</td>
</tr>
<tr>
<td>Adding solvent</td>
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</tr>
<tr>
<td>Simple filtration</td>
<td>0</td>
</tr>
<tr>
<td>Removal of solvent with bp &lt; 150°C</td>
<td>0</td>
</tr>
<tr>
<td>Crystallization and filtration</td>
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<tr>
<td>Removal of solvent with bp &gt; 150°C</td>
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</tr>
<tr>
<td>Solid phase extraction</td>
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<tr>
<td>Distillation</td>
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<tr>
<td>Sublimation</td>
<td>3</td>
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<tr>
<td>Liquid-liquid extraction</td>
<td>3</td>
</tr>
<tr>
<td>Classical chromatography</td>
<td>10</td>
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MEASURING WASTE MINIMIZATION – THE ECO SCALE

<table>
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<td></td>
</tr>
<tr>
<td>Very expen</td>
<td></td>
</tr>
<tr>
<td>3. Safety( ^a )</td>
<td>0</td>
</tr>
<tr>
<td>N (danger)</td>
<td></td>
</tr>
<tr>
<td>T (toxic)</td>
<td></td>
</tr>
<tr>
<td>F (highly flammable)</td>
<td></td>
</tr>
<tr>
<td>E (explosive)</td>
<td></td>
</tr>
<tr>
<td>F+ (extrem)</td>
<td></td>
</tr>
<tr>
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<tr>
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<tr>
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<td>1</td>
</tr>
<tr>
<td>Room temperature, &lt; 24 h</td>
<td>2</td>
</tr>
<tr>
<td>Heating, &lt; 1 h</td>
<td></td>
</tr>
<tr>
<td>Overall Assessment</td>
<td></td>
</tr>
<tr>
<td>Solution</td>
<td>65</td>
</tr>
<tr>
<td>Mechanochemistry</td>
<td>23</td>
</tr>
<tr>
<td>Total Penalty Points</td>
<td>100-65</td>
</tr>
<tr>
<td>EcoScale rating</td>
<td>35</td>
</tr>
<tr>
<td></td>
<td>100-23</td>
</tr>
<tr>
<td></td>
<td>77</td>
</tr>
<tr>
<td>EcoScale rating</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Inadequate</td>
</tr>
<tr>
<td></td>
<td>Excellent</td>
</tr>
<tr>
<td>Overall Assessment</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

SUMMARY

- Risk = hazard x exposure
- Determine scope (use SDS!)
- Assemble your team
- Conduct a hazard assessment
  - Assigning risk ratings
  - Job hazard analysis
- Select controls
- Green engineering principles
- Green chemistry metric: EcoScale

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- Prof. Hairong Guan
- Prof. Neil Ayres

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- Ralph Stuart
- Marta Gmuczyk
- Mary Kirchhoff

Mack Group:
- Heather
- Longrui
- Becca
- Cong
- Joel
- Nina

Undergraduates:
- Preston Carr
- Kingsley Benson

Incoming graduate students:
- Rashad Pace
- Nina Trankina
# Key Chemical Safety References

<table>
<thead>
<tr>
<th>Audience</th>
<th>Technical Resources</th>
<th>Cultural Resources</th>
</tr>
</thead>
<tbody>
<tr>
<td>High school and undergraduate teaching labs</td>
<td><a href="http://example.com">NFPA 45 requirements for instructional and educational labs</a>, 2015</td>
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</thead>
<tbody>
<tr>
<td>Laboratory Researchers</td>
<td>EcoScale green chemistry metric</td>
</tr>
<tr>
<td></td>
<td>ACS Green Chemistry Institute</td>
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<td></td>
<td>“An EcoScale Comparison of Mechanochemistry and Solution Based Reactions,” 2014</td>
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Creating a 21st Century Chemical Research Laboratory: Hazard Assessments and Fundamentals

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“Darren offered a refreshing perspective on how to act as a scientist. It was a nice reminder to find positives in a negative situation. I also liked how Darren challenged the audience to be open to art (and other fields), and not to be a closed-off scientist.”

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