Emerging Opportunities in Chemical Safety Information

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Abstract

- **Abstract:** Public and professional concern about chemical safety in laboratories have mounted over the last decade as a series of incidents in research, teaching and high school settings have led to serious injuries and deaths. In response, several ACS committees and divisions have provided guidance on developing risk assessments for laboratory procedures. However, this strategy faces two specific challenges:
  - 1) convenient access to reliable chemical safety information; and
  - 2) lack of systematic guidance to use this information to identify appropriate hazard management strategies.

- This webinar will describe collaborative efforts between the CINF and CHAS to address these challenges. Specific resources, such as PubChem’s Laboratory Chemical Safety Summaries will be described, as well as logic tools which can support the use of these resources. Opportunities for partnerships for further improving these sources and tools will be discussed.
Today's Topics

1. Overview of Lab Chemistry Safety Logic
2. A Short History of Electronic Lab Safety Information
3. The Librarian's Role in Supporting Safety Logic
4. A Case Study: PubChem LCSSs
5. Getting Involved
6. Looking Forward
Rising Concerns about Chemical Safety in the Lab

The Research Lab

Case Study

Texas Tech University Laboratory Explosion

The Teaching Lab

Safety Bulletin

Key Lessons for Preventing Incidents from Flammable Chemicals in Educational Demonstrations

Creating Safety Cultures in Academic Institutions:

A Report by the Safety Culture Task Force of the ACS Committee on Chemical Safety

The Issue of Laboratory Safety Culture

2011

2012

2014
Are We Learning?

Demonstration methanol fires at:

1. **Beacon School**  
   New York City, January 2014

2. **Discovery Museum**  
   Reno, Nevada, September 2014

3. **STRIVE Preparatory School**  
   Denver, Colorado, September 2014

4. **Cub Scout group**  
   Raymond, Illinois, October, 2014

5. **Lincoln Park High School**  
   Chicago, November, 2014

6. **Lincoln High School**  
   Tallahassee, Florida, May 2015

7. **Woodson High School**  
   Fairfax, VA, November 2015
What Should We Be Learning?

1. **Replacing the Hazard:** use a different demonstration method
2. **Engineering Controls:** in the laboratory, primarily ventilation
3. **Training and Oversight:** for both demonstrators and audience
4. **Personal Protective Equipment:** gloves, glasses or safety shields appropriate to the chemistry and the scenario
5. **Emergency Planning and Response:** both equipment and training

![Image](image_url)

*Figure 3. Methanol igniting on the day of the incident*
The Conceptual Lesson: Safe Chemical Use requires a System

Managing chemical hazards in the lab involves organizing 5 strategies into a system:

1. Hazard Reduction
2. Engineering Controls
3. Training and Oversight
4. Personal Protective Equipment
5. Emergency Planning and Environmental Protection

This approach is appropriate for chemical risks within the scope of the OSHA lab standard. Other uses of chemicals and other hazards require more extensive analysis.
The Reality of the Lab Setting

- Safety in academic research labs is a long standing concern; in 1964, the ACS Committee on Chemical Safety chair wrote: “Scientific research in the campus laboratories is one of the most exciting activities in the world of ideas, and one of the least orderly in the world of organizations.”

- Risk management starts with risk assessment; but lab risks change continuously and unpredictably.

- So we need to develop flexible risk assessment tools and appropriate education for their use.

A recent census of lab hazards at a major research institution; these proportions are changing rapidly.

- Chemicals (80%)
- Biological Agents (40%)
- Radiation (25%)
Emerging Risk Assessment Tools for Lab Hazards

The system is supported by emerging tools. Three key tools are:

– The Globally Harmonized System (GHS)
– The RAMP paradigm from *Laboratory Safety for Chemistry Students* (Hill and Finster) and ACS CPT
– *Identifying and Evaluating Hazards in Research Laboratories* from the ACS
The RAMP model for Building a Lab Safety System

Managing Chemical Safety involves 6 key steps:

1. **EHS Culture**
2. **Hazard Identification**
3. **Risk Assessment**
4. **Managing Safety**
5. **Planning for Emergencies**
6. **Protecting the Environment**

Organizing these tools requires a *partnership* between lab workers and the institution.
The Bottom Line:
Risk Assessment is a Research Process

<table>
<thead>
<tr>
<th>The RAMP model of Chemical Safety</th>
<th>ACRL Information Literacy Skills</th>
</tr>
</thead>
<tbody>
<tr>
<td>Safety culture</td>
<td>Scope the Inquiry</td>
</tr>
<tr>
<td>Recognize hazards</td>
<td>Collect Data</td>
</tr>
<tr>
<td>Assess risks</td>
<td>Evaluate the Information</td>
</tr>
<tr>
<td>Manage safety</td>
<td>Apply Data to Make Decisions</td>
</tr>
<tr>
<td>Plan, Protect Share Lessons Learned</td>
<td>Document the Process and Outcome</td>
</tr>
</tbody>
</table>
In the Real World, Information Systems are Changing As Well

- **1990 – 1998: Web 1.0**
  - data delivery via e-mail and html; **group communication** becomes convenient

- **1998 – 2003: Web 1.5**
  - search engines promote **discovery** and **cross-disciplinary collaboration**

- **2003 – 2010: Web 2.0**
  - So much information is available that information **brokers** are necessary
  - These brokers developed **siloed platforms** to support specific use cases
Examples of Lab Safety Web 2.0 platforms

- **Institutional data:** lab rooms and worker rosters
- **Safety training:** requirements and records
- **Risk data collections:** inventories, SDS’s
- **PPE Wizards**
- **Lab ventilation:** tracking in building management systems
2010 – 2015: Web 2.5

• **Changing technologies**, user **expectations**, and the increasing complexity of the interdisciplinary lab world broke Web 2.0 efforts.

• Part of the reason for this is **poor information management** practices (competing frameworks; poor provenance practices, high training costs) led to unstructured communication that does not **scale**, is not **transferable** between labs and is not **sustainable**.

![Diagram of computer types]  

**Twitter traffic: 2010-2015**
The Vision Beyond 2015

• The emerging web favors:
  – Sites are designed as a **nodes in the network** rather than controllers of the network
  – Consideration of **Contextual Usability** (use of the information beyond the screen)
  – Effective open source **peer curation**, building on e-mail lists and Wikipedia

• What is emerging is a flexibly structured **ecosystem** of **data, workflow tools and domain expertise** mapped to the **essential commonalities** of the use case and content, connected by **good information management practices**
ChemIDplus: A TOXNET DATABASE

Biological Safety Data Sheets

NIOSH Pocket Guide to Chemical Hazards

Does each organization (or scientist) use their own favorite data source(s)?

Do these various data sources provide consistent information (gaps, errors)?

How does the health and safety decision change with different information (or lack of it)?

TOXLINE: A TOXNET DATABASE

Right to Know Hazardous Substance Fact Sheets

CHMINDEX FREE on the WEB!
Many Different Needs

Institutions:
- Research
- Funding
- Regulatory

Stakeholders: Academic View

- Students
- Researchers
- Faculty
- Departments
- Safety Officers
- Librarians

http://www.betterlivingwithreiki.com

LRM
# Laboratory Chemical Safety Summaries

TABLE 1 Information to Be Supplied in Laboratory Chemical Safety Summaries

<table>
<thead>
<tr>
<th>Identifying Information</th>
<th>Name, synonyms, CAS#, and formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical properties</td>
<td>Odor, appearance, water solubility, vapor density, vapor pressure, flash point, autoignition temperature, boiling point (bp) and melting point (mp)</td>
</tr>
<tr>
<td>Toxicity data</td>
<td>Toxicity data is based on exposure in humans, rats, and rabbits through oral, inhaled, and skin exposure.</td>
</tr>
<tr>
<td></td>
<td>LD$_{50}$: Dose of the compound that will cause death in 50% of exposed animals.</td>
</tr>
<tr>
<td></td>
<td>LC$_{50}$: Concentration of the compound that will cause death in 50% of exposed animals (typical for exposure by inhalation).</td>
</tr>
<tr>
<td></td>
<td>LC$_{10}$: Lowest concentration of a compound reported to cause death in humans or animals.</td>
</tr>
<tr>
<td>Exposure limits</td>
<td>REL: NIOSH-recommended exposure limit.</td>
</tr>
<tr>
<td></td>
<td>STEL/ceiling: Short-term exposure limit, maximum concentration an individual can be exposed to for a period of 15 minutes.</td>
</tr>
<tr>
<td></td>
<td>PEL: OSHA permissible exposure limits, maximum concentration of a chemical in air based on a 8-hour weighted average.</td>
</tr>
<tr>
<td></td>
<td>TLV-TWA: ACGIH threshold limit value-time weighted average.</td>
</tr>
<tr>
<td>Health and symptoms</td>
<td>The “General” statement summarizes the broad implication of exposure and includes a statement on the potential for odor to act as an indicator for the presence of the molecule (or warning for overexposure). Additional health risks and symptoms are categorized by routes of exposure (skin, eye, ingestion, and inhalation).</td>
</tr>
<tr>
<td>First aid</td>
<td>Categorized by routes of exposure (skin, eye, ingestion, and inhalation).</td>
</tr>
<tr>
<td>Flammability and explosivity</td>
<td>NFPA ratings for flammability</td>
</tr>
<tr>
<td></td>
<td>0: Material will not burn.</td>
</tr>
<tr>
<td></td>
<td>1: Material must be preheated before ignition can occur.</td>
</tr>
<tr>
<td></td>
<td>2: Material must be moderately heated or exposed to relatively high ambient temperature before ignition can occur.</td>
</tr>
<tr>
<td></td>
<td>3: Liquids or solids can be ignited under almost all ambient temperature conditions.</td>
</tr>
<tr>
<td></td>
<td>4: Materials will rapidly or completely vaporize at atmospheric pressure and normal ambient temperature, or are readily dispersed in air and will burn readily.</td>
</tr>
<tr>
<td></td>
<td>LEL: Lower explosive limit: lowest concentration of a gas or a vapor in air that will burn in presence of an ignition source.</td>
</tr>
<tr>
<td></td>
<td>UEL: Upper explosive limit: highest concentration of a gas or a vapor in air that will burn in presence of an ignition source.</td>
</tr>
<tr>
<td>Reactivity and incompatibility</td>
<td>Describe which chemicals will produce an undesirable chemical reaction or degradation when mixed with the title compound.</td>
</tr>
<tr>
<td>Storage and handling</td>
<td>General guidelines for the storage and handling of chemicals along with recommendations for the use of personal protective equipment and clothing have been outlined in Chapter 6. For guidance on the selection and use of ventilators, consult OSHA regulation 29 CFR § 1910.134.</td>
</tr>
<tr>
<td></td>
<td>Gloves: Latex gloves are typically suitable for use with most chemicals when using prudent practices. Gloves suggested herein are those deemed to be least permeable by the named chemical during incidental chemical contact. Gloves should be selected that are best for the application. See a glove selection guide for additional criteria to consider when selecting a glove.</td>
</tr>
<tr>
<td>Cleanup and disposal</td>
<td>Additional information on the cleanup and disposal of hazardous waste is given in Chapter 8.</td>
</tr>
<tr>
<td>Additional considerations</td>
<td>A few notations have been made to identify chemicals that can act as suitable replacements for substances with harsh environmental impacts. Additional information on alternative chemicals and synthetic approaches may be found on the EPA Web site.</td>
</tr>
<tr>
<td></td>
<td>Chemicals that are not appropriate for use with students K-12 or first-year science students at the undergraduate level have been identified based on recommendations compiled by the American Chemical Society’s Joint Board–Council Committee on Chemical Safety. Chemicals not appropriate for use with students may be highly explosive or flammable or have extremely unfavorable health implications or possess a significant risk larger than the intended academic benefit.</td>
</tr>
</tbody>
</table>
Data Source of Data Sources

By integrating these, PubChem acts as a one stop shop for data needs with links back to primary data sources.

One chemical .. many useful sources
Each resource has some overlaps
Each resource has unique content

What if you have ten chemicals?
What if you have ten sources for each?
How much time will one spend comparing these?
# Laboratory Chemical Safety Summary (LCSS) Form (NRC)

## NAME
acetone

### SYNONYMS [synonyms]
- [top header, 3.3]

### CAS® Formula
- [top header, 3.2.1]

## PHYSICAL PROPERTIES [experimental properties]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Odor</td>
<td>4.2</td>
</tr>
<tr>
<td>Water Solubility</td>
<td>4.28</td>
</tr>
<tr>
<td>Flash Point</td>
<td>4.27</td>
</tr>
<tr>
<td>Autoignition</td>
<td>4.2.13</td>
</tr>
<tr>
<td>Vapor Pressure</td>
<td>4.2.11</td>
</tr>
</tbody>
</table>

## TOXICITY [toxicological information]

### EXPOSURE LIMITS [safety and hazard properties]

<table>
<thead>
<tr>
<th>Exposure</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>LD50 oral</td>
<td>10.1.8</td>
</tr>
<tr>
<td>LC50 inhalation</td>
<td>10.1.8</td>
</tr>
<tr>
<td>LD50 skin</td>
<td>10.8</td>
</tr>
</tbody>
</table>

## HEALTH AND SYMPTOMS [hazard identification] [toxicological information]

### General | 9.1.2-10.12, 10.1.2 |
### Skin    | 9.1.7.12 |
### Eyes    | 9.1.9.12 |
### Ingestion | 9.1.10.12 |
### Inhalation | 9.1.8.12 |

## FIRST AID [first aid measures]

### Skin    | 9.3.1.5 |
### Eyes    | 9.3.1.6 |
### Ingestion | 9.3.1.7 |
### Inhalation | 9.3.1.4 |

## FLAMMABILITY & EXPLOSION [safety and hazard properties], [fire fighting measures], [first aid measures]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>NFPA rating (flammability)</td>
<td>9.2.13</td>
</tr>
<tr>
<td>CEL (i.e., flash point)</td>
<td>9.2.1</td>
</tr>
<tr>
<td>UEL (i.e., upper explosive limit)</td>
<td>9.2.2</td>
</tr>
</tbody>
</table>

## REACTIVITY & INCOMPATIBILITY [reactivities and incompatibilities], [properties - chemical dangers]

<table>
<thead>
<tr>
<th>Reactivity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage and Handling</td>
<td>[exposure control and personal protection], [handling and storage], [accidental release - other preventative measures]</td>
</tr>
</tbody>
</table>

## CLEANUP & DISPOSAL [accidental release measures], [handling - nonfire spill response]

<table>
<thead>
<tr>
<th>Cleanup and Disposal</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Additional Considerations</td>
<td>[Toxic Combustible Products], [Other Hazardous Reactions]</td>
</tr>
</tbody>
</table>

## Data in PubChem Laboratory Chemical Safety Summary (LCSS)

- As of October 30, 2015
- Abbreviations in brackets indicate data sources.

### GHS Classification [CLP, GHS]
- Symptom [NOSH]
- Target ORG [ATSDR, NIOSH]
- Sensory Effects [ICSC, NIOSH]
- Toxicology [ICSC, NIOSH]
- Skin Care [NIOSH]
- Health Hazards Summary [ATSDR, EPA-AT, NIOSH]
- Inorganic Key [PC]

### Physical Properties
- Physical Description [CAMEO, EPA-CDR, ICSC, NIOSH, OSHA]
- Odor [OSHA]
- Flash Point [ICSC, NIOSH]
- Melting Point [ICSC, NIOSH]
- Solubility [ICSC, NIOSH]
- Vapor Pressure [ICSC, NIOSH]
- Auto-Ignition [ICSC, ICSC]
- Corrosivity [ICSC]
- Toxicity Data
  - Acute Oral LD50, LD50 Skin, LC50 Inhalation
  - Skin: LD50, LC50
  - Eyes: EC50

### Flammability and Explosivity
- Flammability [OSHA]
- Lower Explosive Limit (UEL) [OSHA]
- Upper Explosive Limit (UEL) [OSHA]
- NFPA: Hazard Classification (ICSC)
- NFPA Fire Rating (ICSC)
- NFPA Reactivity Rating (ICSC)
- NFPA Health Rating (ICSC)
- NFPA Other (ICSC)

### Storage and Handling
- Storage and Disposal [ICSC, NIOSH]
- Personal Protective Equipment (PPE) [ICSC]
- Respirator Recommendations [NIOSH]
- Spillage Response [OSHA]
- Disposal Methods (HSDR)

### Additional Considerations
- Toxic Combustible Products [HSDR]
- Other Hazardous Reactions [HSDR]
Benzene

3.3 Boiling Point

80.08 deg C


176.2 °F (at 760 mmHg)
(NTP, 1992)

200 to 500 °F (at 760 mmHg)
(USCG, 1999)

Source Name: CAMEO Chemicals
Source ID: CBNOAA0000000002577
Record Name: Benzene
URL: http://cameochemicals.noaa.gov/chemical/2577

Source Name: CAMEO Chemicals
Source ID: CBNOAA00000000001158
Record Name: Coal tar oil, heavy distillate
URL: http://cameochemicals.noaa.gov/chemical/1158

Read about the LCSS project ♦

Cite this Record
Finding LCSSs at PubChem

PubChem LCSS as a data stream


Safety Office Use Cases

- Inventory systems (consolidated data stream)
- Chemical profiling (safety planning)
  - incident analysis
  - reactivity classification
- Research tool for safety system studies
- The system will be used to provide suggestions for safety measures.

Inventory Requirements:
- GHS labeling with pictograms, signal words and hazard statement codes
- SDS from manufacturer or equivalent for ‘house solutions’ (including incompatibilities)
- Identifiers, preferably with concentration and physical form specification
Chemistry Educator Use Cases

• Chemical profiling for lab curriculum (download LCSSs for chemical lists)
• Teaching literacy in RAMP process (searching for information and comparing data sources)
• Analyzing procedures for chemical, equipment and process hazards

ChemicalTagger

- University of Cambridge > Department of Chemistry > Unilever Centre for Molecular Science Informatics

**Di-tert-butylphosphinoferrocene.** An oven-dried **1000-mL four-necked** (one 34/45 joint and three 24/40 joints) round-bottomed flask is allowed **to cool in a desiccator over anhydrous calcium sulfate.** Once cool, the central joint is equipped with an overhead mechanical stirrer, the glass rod of which is fitted with 7.2 x 2 cm **Teflon** paddle, coated with lubricant (Note 1), and sheathed by a 34/45 jointed glass stirrer bearing. The remaining three necks are fitted with a thermocouple in a 24/40 adapter, an argon line connected to a 24/40 adapter, and rubber septum. The rubber septum is removed from the fourth neck and the flask is charged with ferrocene (8.0 g, 43.0 mmol, 1 equiv.) (Note 2). A **250-mL pressure-equalizing addition funnel with a 24/40 joint** is fitted in the fourth neck and the reaction set-up is flushed with argon for 5 min (see Note 3 for an image of the reaction setup).

- **Actions:**
  - [x] Degass
  - [ ] ApparatusAction
  - [ ] Apparatus
  - [ ] Conditions
  - [ ] TimePhrase
  - [ ] Molecules
  - [x] Other
Chemistry Researcher Use Cases

- Experimental planning
- Capturing lab risk assessments and any lessons learned
- Publication of safety notes as part of Supplemental Information
- Use of safety info tools and documentation promotes safe research group culture

Need for Targeted Information:
- Identification of reagents, products
- Reactivity and associated hazard analysis
- Associated exposure control information
- Alternative reagents or reaction pathways
- Iterative over repeated experiments

Caution! tert-Butyllithium is extremely pyrophoric and must not be allowed to come into contact with the atmosphere. This reagent should only be handled by individuals trained in its proper and safe use. It is recommended that transfers be carried out by using a 20-mL or smaller glass syringe filled to no more than 2/3 capacity or by cannula. For a discussion of procedures for handling air-sensitive reagents, see Aldrich Technical Bulletin AL-134.
Chemical Vendor Use Cases

- Requirement to disseminate chemical safety information (e.g., SDS)
- Visibility of catalog information
Information Practices that Support this Vision

• **Ontology**: the machine readable system of definitions and links between those definitions

• **Annotation**: the human process of prioritizing elements and making decisions based on the available resources and the goal of the project
Information Practices that Support this Vision

• What does this give you?
  – Improved query / analysis
    Go to a web search engine
    Type in a natural language query
    Get an answer

  What is the boiling point of benzene?
Call to Action!

- Professional Safety Community
- Chemical Educator Community
- Chemical Information Community
  - Information Scientists
  - Librarians & Service Providers
Safety Professional Input

• Data
  – What is needed/available or should be added/removed?

• Use
  – Are data access mechanisms/formats appropriate?

• Review
  – Is anything amiss? Chemical use case variation?

• Annotation
  – Share your annotation and help improve that available

• Tell a friend
  – Expanding the community will increase impact
• Common chemical lists and lab procedures
  – Are they covered?
  – Mixtures vs. pure chemicals?

• RAMP exercises to model
  – Is the information available to support Risk Assessments as they are practiced and taught?

• Considerations unique to non-research lab exercises and demonstrations?
Cheminformaticians...

- Data ingest, management, structure
- Grouping/classification, terminology/synonymy
- Text mining & analysis
- Clean, sanitize, validate
- Do the above ...
  or else... (horror!)
Chemistry Librarians

• Suggest data sources
  – MORE MORE MORE!!!

• Develop safety data re-use scenarios
  – Outline services, including annotation
  – Document instructions for accessing data
  – Assist in establishing use in various institutions
    • Teaching labs
    • Research labs, ELN systems, etc.
    • EHS and other campus service offices

• Promote Literacy
  – Promoting awareness and use of sources
  – Encouraging evaluation of data and provenance
Related Information Efforts

• IUPAC InChI projects
  – QR code (integrated with barcode scanners)
  – Mixtures extension (purity, components, etc.)
  – Lookup service (protocols for federated search)
• Pistoia Chemical Safety Library initiative
• Others (often with variable use cases)
Future Work

1. Develop **process descriptors** which can data mine the literature to identify process hazards (CINF professionals)
2. Develop a **Chemical Safety Ontology** (joint effort of CINF and EHS professionals)
3. Develop a **crowd annotation** approach for EHS professionals, potentially hosted by PubChem, an institution and/or service (TBD)
4. **Lessons learned** framework
The Future: Ongoing Collaboration with a Variety of Partners

General news about the project's progress can be found at [http://www.irampp.org](http://www.irampp.org)
   http://confchem.ccce.divched.org/2015FallCCCENLP3
   http://pubs.acs.org/doi/abs/10.1021/acs.jchemed.5b00511
Thanks to Many Colleagues!

- American Chemical Society (ACS) Professional Member Divisions of Chemical Health & Safety (CHAS), Chemical Information (CINF), Chemical Education (CHED)
- ACS Committee on Chemical Safety (CCS) Safety Advisory Panel (SAP)
- National Library of Medicine (NLM) PubChem Team
- Institutional Collaborators
  - University of California
  - University of New Hampshire
Questions?