BUILDING AN ECOSYSTEM OF CHEMICAL SAFETY INFORMATION

Leah McEwen
Cornell University

Ralph Stuart
Keene State College

ACS Presidential Symposium on Chemical Safety

Boston 2018

[Feb Safety Summit]

American Chemical Society

ACS Chemistry for Life™

2018 ACS Safety Summit:
Bringing
Professionalism, Safety and Ethics
to
Chemistry for Life™

Ralph Stuart, Chair
Committee on Chemical Safety

Dr. Dorhout's Goals for the ACS Safety Culture Summit

ACS Chemistry for Life™

1. Coordinate *ACS efforts and expertise* in the area of chemical safety, with a focus on **safety culture** in academic laboratories.
2. Formulate *future ACS strategy* to demonstrate the Society's leadership in advancing a **culture of safety** in the chemical enterprise.
3. Engage ACS *stakeholders and external experts* in the chemical safety conversation to promote an **ethos of safety.**
4. Identify *tools, opportunities, and partnerships* that ACS can leverage to support **safety cultures**.

Cultures are historically bound, so let's take a quick look back at ACS chemical safety strategies in the 20th Century.

[Summit Outcomes]

The Summit's Starting Point:

ACS Chemistry for Life

ACS Chemistry for Life

STRATEGIC PLAN
for 2018 and Beyond

Vision

Improving people's lives through the transforming power of chemistry

Mission

Advancing the broader chemistry enterprise and its practitioners for the benefit of Earth and its people

ACS Overall Strategic Goals

1. Provide Information Solutions
2. Empower Members and Member Communities
3. Support Excellence in Education
4. Communicate Chemistry's Value

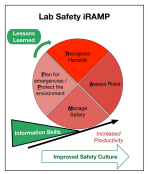
American Chemical Society

Strategic Opportunities in Chemical Safety for ACS

ACS Chemistry for Life

1. Develop Safety Information Solutions

Develop specific use cases for RAMP



Stakeholder Workshops

2. Empower Members with Safety Skills

3. Support Safety Education

RAMP outreach

4. Communicate Chemical Safety as a Core Value

Support the ecosystem of professional safety resources

American Chemical Society 9

[SAP June]

ACS Safety Programs

Division of Chemical Health and Safety
- National and Regional Meeting technical programs
- *J of Chemical Health and Safety* and DCHAS-L e-mail list
- Professional Development Workshops
- Innovative Project Grants
- Technical division partnerships .particularly CHED and CINF

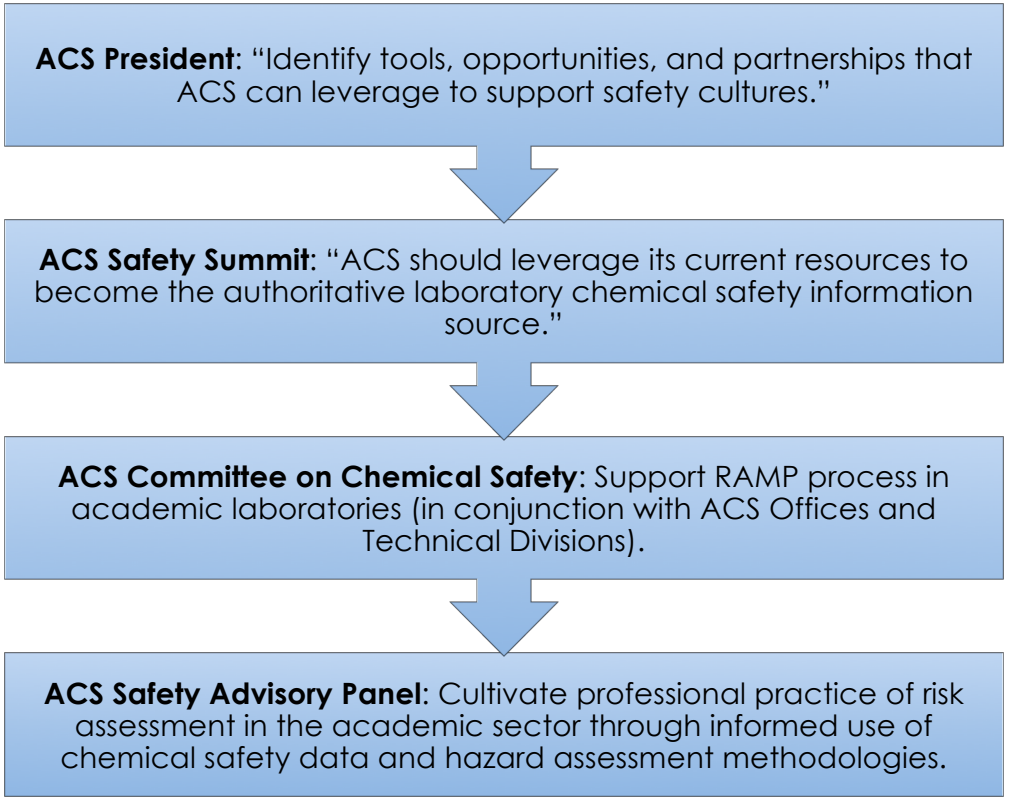
Committee on Chemical Safety
- Education Subcommittee
- Communication Subcommittee
- Safe Practices Subcommittee
- **Safety Advisory Panel**

ACS Safety Program Office Coordination
- NSTA outreach
- CPSC support on flame-jetting education
- ACS Regional meeting workshops
- Document library maintenance
- Support for ACS outreach staff on safety issues

2018 Strategic Tasks for the Safety Advisory Panel

ACS Strategic Audiences	SAP topics
Members and potential members	Risk assessment documentation tools
Educators	Risk assessment teaching tools
Decision-makers	Chemical safety information policy issues
The Public, especially STEM high school students	Developing the connection between Chemical Safety and Green Chemistry (and Chemical Security?)

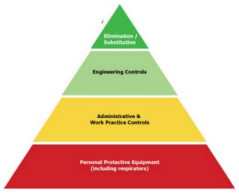
INFORMATION GOALS FOR SAFETY



Lab safety involves technical and cultural skills

Selecting Controls Based on Rules, guided by Chemical Intuition

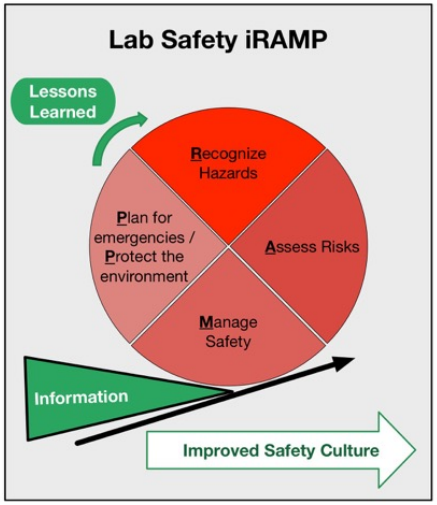
Manage Hazards



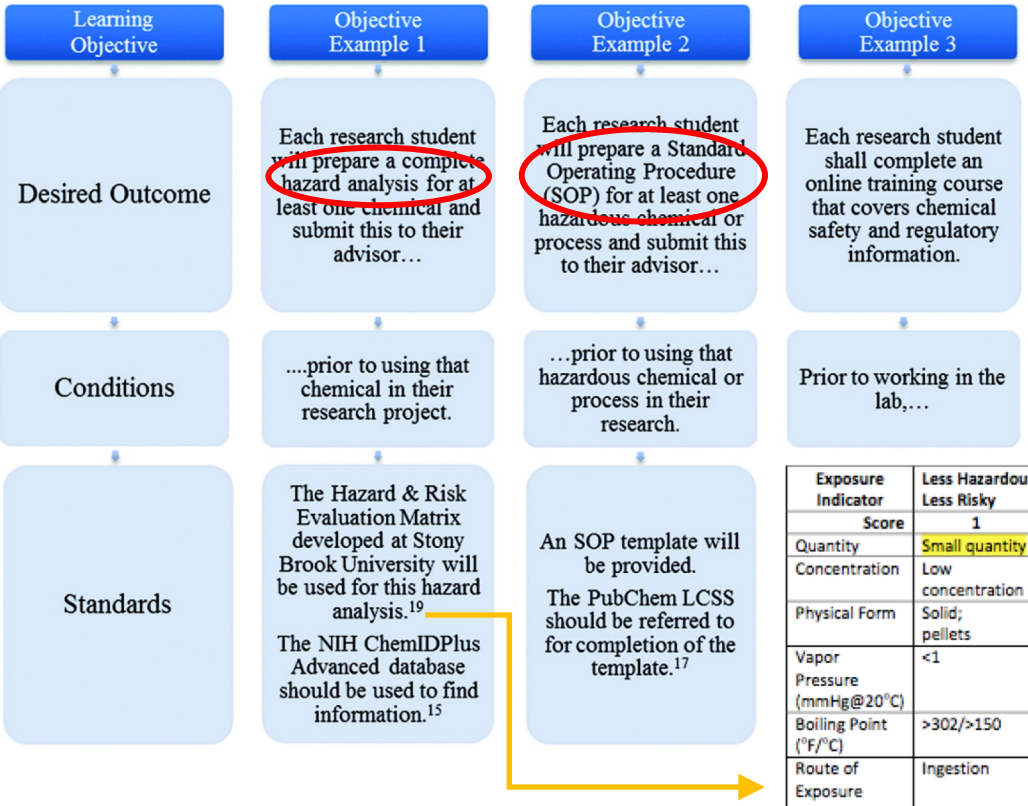
OSHA Controls

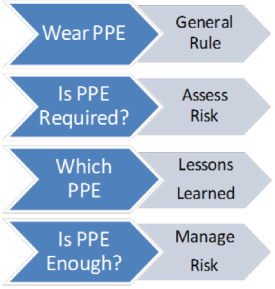
Culture Change through Safety Education

Safety System based on documented Risk Assessment



Learning Objectives





Exposure Indicator	Less Hazardous Less Risky				More Hazardous More Risky	Score
Score	1	2	3	4	5	
Quantity	Small quantity		Intermediate quantity		Large quantity	1
Concentration	Low concentration		Intermediate concentration		High concentration	5
Physical Form	Solid; pellets	Liquids; granules	Mists	Vapors/fumes; Fine powders	Gas; Nanoparticles	2
Vapor Pressure (mmHg@20°C)	<1	1 – 10	>10 – 100 [@ 25]	>100 – 760	>760	3
Boiling Point (°F/°C)	>302/>150		122 – 302/50 – 150		<122/<50	3
Route of Exposure	Ingestion		Skin contact and ingestion		Inhalation, skin contact and ingestion	5
Detection	Appearance	Established odor/irritation levels	Odor/irritation threshold	Odor/irritation levels not established	Analytical methods	2
Warning Properties	Odor/irritation threshold is below PEL/TLV (0.75 < 2-2.5)			Odor/irritation threshold is above PEL/TLV		1
				Add all above scores	Exposure Score	22

Sigmann and McEwen, 2016
DOI: 10.1021/bk-2016-1232.ch003

Hazard Assessment Paper Tools

	Job Hazard Analysis			
Step	**Work Steps and Tasks** *Describe the tasks / steps involved in the work – in order*	**Hazards Identified for each Task / Step**	**Risk Level (exposure x probability x consequence)** *Risk Nomogram used*	**Control / Safe Work Procedures for each Task / Step** *Controls to be implemented*
…				
5	Remove stock bottle of concentrated nitric acid from storage	**Chemical splash – Corrosive; eye & skin damage; inhalation (toxic gas); Chemical spill; Oxidizing liquid**	**Moderate >20, but < 50**	**Nitric acid is very reactive. Do not underestimate this hazard. Include and review SDS as a control in this JHA. Wear all PPE as above, HOWEVER nitrile does not protect well for concentrated acid – double glove, add polyethylene or butyl rubber Note location of and visually inspect spill kit w/ neutralizing material Review ER procedures If large spill occurs i.e. 2.5 L bottle, evacuate and notify**
6	Transfer ~50 mL of con nitric to 250 beaker	**Same as step 5**	**Moderate >20, but < 50**	**Same as step 5**
7	Return stock bottle of concentrated nitric acid to storage	**Same as step 5**	**Moderate >20, but < 50**	**Same as step 5**
8	Add 30 mL of concentrated nitric acid (16 M HNO_3) Stir as needed	**Chemical splash – corrosive; eye damage; inhalation (NO_2, toxic gas) Chemical spill Oxidizing liquid**	**Low <10**	**Wear all PPE as above, HOWEVER nitrile does not protect well for concentrated acid – double glove, add polyethylene or butyl rubber WORK IN FUME HOOD – lower sash; set up at least 6" inside Stir slowly with magnet on stir plate to displace nitrogen dioxide (NO_2) a toxic brown gas. Cover with watch glass if needed. Beaker graduations offer sufficient accuracy, so minimize cleaning by not measuring with other equipment.**

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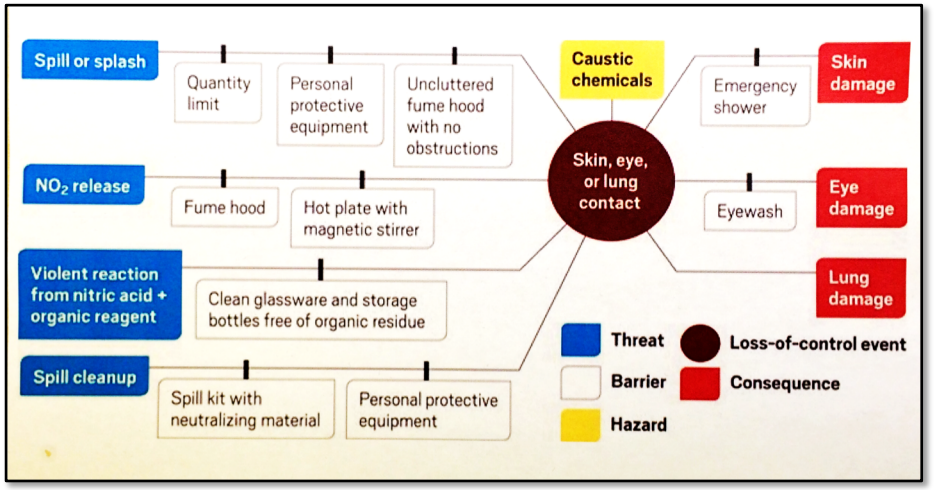


SDS:
core information source for hazard recognition

OSHA® QUICK CARD™

Hazard Communication Standard Pictogram

The Hazard Communication Standard (HCS) requires pictograms on labels to alert users of the chemical hazards to which they may be exposed. Each pictogram consists of a symbol on a white background framed within a red border and represents a distinct hazard(s). The pictogram on the label is determined by the chemical hazard classification.

HCS Pictograms and Hazards

Health Hazard  • Carcinogen • Mutagenicity • Reproductive Toxicity • Respiratory Sensitizer • Target Organ Toxicity • Aspiration Toxicity	**Flame**  • Flammables • Pyrophorics • Self-Heating • Emits Flammable Gas • Self-Reactives • Organic Peroxides	**Exclamation Mark**  • Irritant (skin and eye) • Skin Sensitizer • Acute Toxicity (harmful) • Narcotic Effects • Respiratory Tract Irritant • Hazardous to Ozone Layer (Non-Mandatory)
Gas Cylinder  • Gases Under Pressure	**Corrosion**  • Skin Corrosion/ Burns • Eye Damage • Corrosive to Metals	**Exploding Bomb**  • Explosives • Self-Reactives • Organic Peroxides
Flame Over Circle  • Oxidizers	**Environment** (Non-Mandatory)  • Aquatic Toxicity	**Skull and Crossbones**  • Acute Toxicity (fatal or toxic)

For more information:

U.S. Department of Labor

OSHA Occupational Safety and Health Administration

www.osha.gov (800) 321-OSHA (6742)

OSHA 3491-01R 2016

OSHA® QUICK CARD™

Hazard Communication Safety Data Sheets

The Hazard Communication Standard (HCS) requires chemical manufacturers, distributors, or importers to provide Safety Data Sheets (SDSs) (formerly known as Material Safety Data Sheets or MSDSs) to communicate the hazards of hazardous chemical products. The HCS requires new SDSs to be in a uniform format, and include the section numbers, the headings, and associated information under the headings below:

Section 1, Identification includes product identifier; manufacturer or distributor name, address, phone number; emergency phone number; recommended use; restrictions on use.

Section 2, Hazard(s) identification includes all hazards

Section 3, Composition/information on ingredients includes information on chemical ingredients; trade secret claims.

Section 4, First-aid measures includes important symptoms/effects, acute, delayed; required treatment.

Section 5, Fire-fighting measures lists suitable extinguishing techniques, equipment; chemical hazards from fire.

Section 6, Accidental release measures lists emergency procedures; protective equipment; proper methods of containment and cleanup.

Section 7, Handling and storage lists precautions for safe

(Continued on other side)

For more information:

U.S. Department of Labor

OSHA Occupational Safety and Health Administration

www.osha.gov (800) 321-OSHA (6742)

OSHA 3493-01R 2016

OSHA® QUICK CARD™

Hazard Communication Safety Data Sheets

Section 8, Exposure controls/personal protection

ACGIH Threshold Limit Values (TLVs); and any other exposure limit used or recommended by the chemical manufacturer, importer, or employer preparing the SDS where available as well as appropriate engineering controls; personal protective equipment (PPE).

Section 9, Physical and chemical properties lists the chemical's characteristics.

Section 10, Stability and reactivity lists chemical stability

Section 11, Toxicological information includes routes of exposure; related symptoms, acute and chronic effects; numerical measures of toxicity.

Section 13, Disposal considerations*

Section 15, Regulatory information*

Section 16, Other information, includes the date of preparation or last revision.

*Note: Since other Agencies regulate this information, OSHA will not be enforcing Sections 12 through 15 (29 CFR 1910.1200(g)(2)).

Employers must ensure that SDSs are readily accessible to employees.
See Appendix D of 29 CFR 1910.1200 for a detailed description of SDS contents.

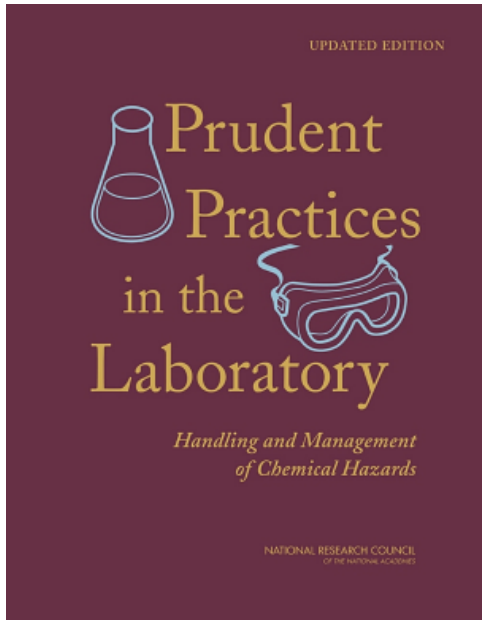
For more information:

U.S. Department of Labor

OSHA Occupational Safety and Health Administration

www.osha.gov (800) 321-OSHA (6742)

Prudent Practices –>
Laboratory Chemical Safety Summaries



NAME

SYNONYMS [synonyms]	**CAS#**	**Formula**
[top header, 3.3]	[top header, 3.2.1]	[top header]

PHYSICAL PROPERTIES [experimental properties]			
Odor: [4.2.3, 4.219]		**Appearance:**	[top header, 4.2.1]
Water Solubility: [4.2.8]		**Vapor Density:**	[4.2.10]
Flash Point: [4.2.7]		**Vapor Pressure:**	[4.2.11]
Autoignition: [4.2.13]		**bp/mp:**	[4.2.5]/ [4.2.6]
TOXICITY [toxicological information]		**EXPOSURE LIMITS [safety and hazard properties]**	
LD_{50} oral ( )	[10.1.8]	**TLV-TWA (ACGIH)**	[9.2.18], [9.2.26]
LC_{50}inhal. ( )	[10.1.8]	**STEL (ACGIH)**	[9.2.26]
LD_{50} skin ( )	[10.1.8]	**PEL (OSHA)**	[9.2.5]

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 & EXPLOSIVITY
[safety and hazard properties],[fire fighting measures],[first aid measures]
[9.2.9] NFPA rating (flammability) = [9.2.13]; LEL = [9.2.1]; UEL = [9.2.2]
[9.4], [9.3.2,3], [9.2.16]

REACTIVITY & INCOMPATIBILITY
[reactivities and incompatibilities],[properties - chemical dangers]
[9.8], [9.2.17]

STORAGE & HANDLING [exposure control and personal protection],[handling and storage],[accidental release - other preventative measures]
[9.7], [9.6], [9.5.4]

CLEANUP & DISPOSAL
[accidental release measures],[handling - nonfire spill response]
[9.5], [9.6.1]

ADDITIONAL CONSIDERATIONS

NextGen LCSS

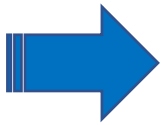
Data contents in PubChem
Laboratory Chemical Safety Summary (LCSS)

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

GHS Classification [CLP, ICSC]
Synonyms [PC]
Identifiers
PubChem CID [PC]
CAS [DRGBNK, EPA-CDR, ICSC, NIOSH, OSHA]
InChI [PC]
InChI Key [PC]
Physical Properties
Physical Description [CAMEO, EPA-CDR, ICSC, NIOSH, OSHA]
Odor [HSDB]
Boiling Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
Melting Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
Flash Point [HSDB, ICSC, NIOSH, OSHA]
Solubility [CAMEO, DRGBNK, HSDB, ICSC, NCI, NIOSH]
Density [CAMEO, HSDB, ICSC, NIOSH, OSHA]
Vapor Density [CAMEO, HSDB, ICSC, OSHA]
Vapor Pressure [CAMEO, HSDB, ICSC, NIOSH, OSHA]
Auto-Ignition [HSDB, ICSC]
Decomposition [HSDB, ICSC]
Corrosivity [HSDB]
Odor Threshold [HSDB]
Toxicity Data
Toxicity Summary [DRGBNK, HSDB]
Human Toxicity Values [HSDB]
Non-Human Toxicity Values [HSDB]
Exposure Limits
Immediately Dangerous to Life or Health Concentration [NIOSH, OSHA]
Recommended Exposure Limit (REL) [NIOSH, OSHA]
Permissible Exposure Limit (PEL) [NIOSH, OSHA]
REL-Time-Weighted Average Concentration (REL-TWAC) [OSHA]
REL-Short-Term Exposure Limit (REL-STEL) [OSHA]
REL-Ceiling (REL-C) [OSHA]
PEL-Time-Weighted Average Concentration (PEL-TWAC) [OSHA]
PEL-Short-Term Exposure Limit (PEL-STEL) [OSHA]
PEL-Ceiling (PEL-C) [OSHA]
Threshold Limit Values [HSDB]
Occupational Exposure Limits [ICSC]
Effects of Short Term Exposure [ICSC]
Effects of Long Term Exposure [ICSC]
Explosive Limits and Potential [HSDB, ICSC]
Radiation Limits and Potential [HSDB]
Acceptable Daily Intakes [HSDB]
Allowable Tolerances [HSDB]
Health and Symptoms
Symptoms [NIOSH]
Carcinogen [ATSDR, HSDB, OSHA]
Exposure Routes [ICSC, NIOSH]
Target Organs [ATSDR, NIOSH]
Cancer Sites [NIOSH]
Fire Hazard [ICSC]
Explosion Hazard [ICSC]
Exposure Hazard [ICSC]
Skin Hazard [ICSC]
Inhalation Hazard [ICSC]
Eye Hazard [ICSC]
Ingestion Hazard [ICSC]
Hazards Summary [ATSDR, EPA-AT, HSDB]
Fire Potential [HSDB]
Skin, Eye, and Respiratory Irritations [HSDB]
First Aid
Fire First Aid [ICSC]
Explosion First Aid [ICSC]
Exposure First Aid [ICSC]
Inhalation First Aid [ICSC]
Skin First Aid [ICSC]
Eye First Aid [ICSC]
Ingestion First Aid [ICSC]
Flammability and Explosivity
Flammability [HSDB, NIOSH]
Lower Explosive Limit (LEL) [NIOSH, OSHA]
Upper Explosive Limit (UEL) [NIOSH, OSHA]
NFPA Hazard Classification [HSDB]
NFPA Fire Rating [CAMEO, OSHA]
NFPA Reactivity Rating [CAMEO, OSHA]
NFPA Health Rating [CAMEO, OSHA]
NFPA Other [CAMEO, OSHA]
Critical Temperature [HSDB]
Critical Pressure [HSDB]
Stability and Reactivity
Reactivities and Incompatibilities [HSDB, NIOSH, OSHA]
Storage and Handling
Safe Storage [ICSC]
Storage Conditions [HSDB]
Protective Equipment and Clothing [HSDB]
Personal Protection [NIOSH]
Respirator Recommendations [NIOSH]
Nonfire Spill Response [OSHA]
Cleanup and Disposal
Spillage Disposal [ICSC]
Cleanup Methods [HSDB]
Disposal Methods [HSDB]
Additional Considerations
Toxic Combustion Products [HSDB]
Other Hazardous Reactions [HSDB]

Data Source Abbreviations

- ATSDR = CDC ATSDR Toxic Substance Portal
- CAMEO = NOAA CAMEO Chemicals
- CLP = Regulation (EC) No 12 1272/2008
- DRGBNK = DrugBank
- EPA-AT = EPA Air Toxics
- EPA-CDR = EPA Chemical Data Report
- HSDB = Harzardous Substances Data Bank
- ICSC = ILO International Chemical Safety Cards
- NCI-ID = NCI Investigational Drugs
- NIOSH = NIOSH Pocket Guide
- OSHA = OSHA Occupational Chemical DB
- PC = PubChem



NIH › NLM › NCBI

PubChem OPEN CHEMISTRY DATABASE

Search Compounds

LCSS Laboratory Chemical Safety Summary for CID 180 — Download | Print | Share | Help

PUBCHEM › COMPOUND › ACETONE › LCSS — *Read about the LCSS project*

Acetone

Cite this Record

PubChem CID:	180
Chemical Names:	Acetone; 2-propanone; Propanone; Dimethyl ketone; Methyl ketone; 67-64-1
Molecular Formula:	C_3H_6O or CH_3-CO-CH_3 or $(CH_3)_2CO$
Molecular Weight:	58.07914 g/mol

Contents

1 GHS Classification

Signal: Danger
GHS Hazard Statements
H225: Highly Flammable liquid and vapor [Danger Flammable liquids - Category 2]
H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation - Category 2A]
H336: May cause drowsiness or dizziness [Warning Specific target organ toxicity, single exposure; Narcotic effects - Category 3]
Precautionary Statements
P210: Keep away from heat, hot surface, sparks, open flames and other ignition sources. - No smoking.
P233: Keep container tightly closed.
P240: Ground/bond container and receiving equipment.

SAP identified two areas of work focus:

1. **Design online RAMP tools for different use cases**
   - what are the data and functionality criteria for online tools that support the process of risk assessment in teaching labs (e.g., organic)?
   - can we develop preformulated RAMP “cake mixes” of safety data and scale-specific procedures to facilitate risk assessment for specific contexts (e.g., substitute rainbow demonstration setup)
2. **Curation of data sources**
   - academic community needs a laboratory scale SDS-like data format, what about the LCSS from Prudent Practices?
   - do we have the right data? do we have the right authoritative sources?
   - can this data be ingested and integrated into other information systems to be more accessible in user workflows?

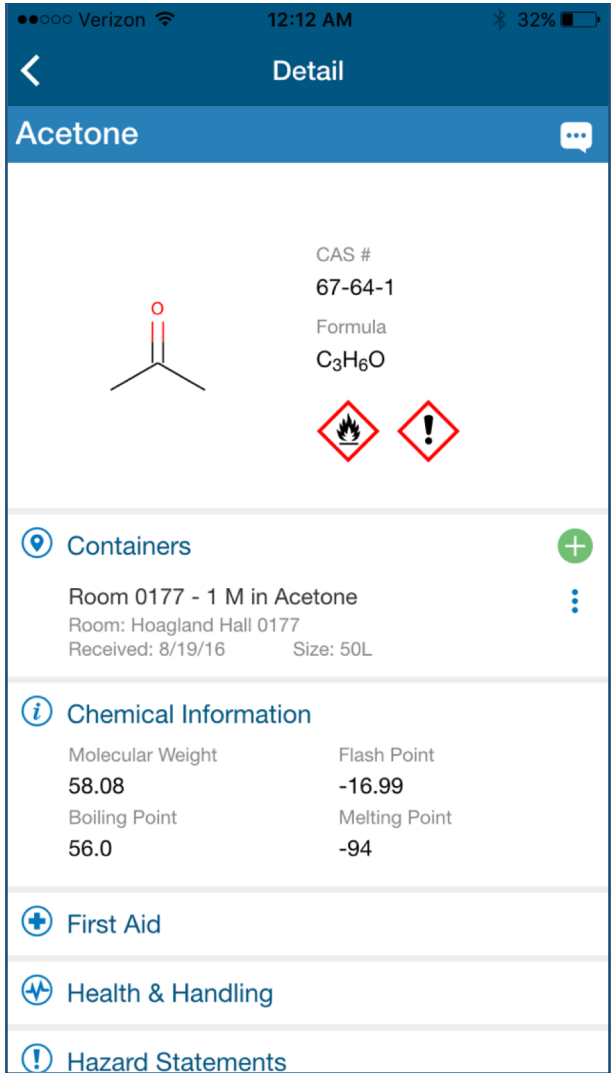
IPG: proof-of-concept **interactive RAMP e-tool**

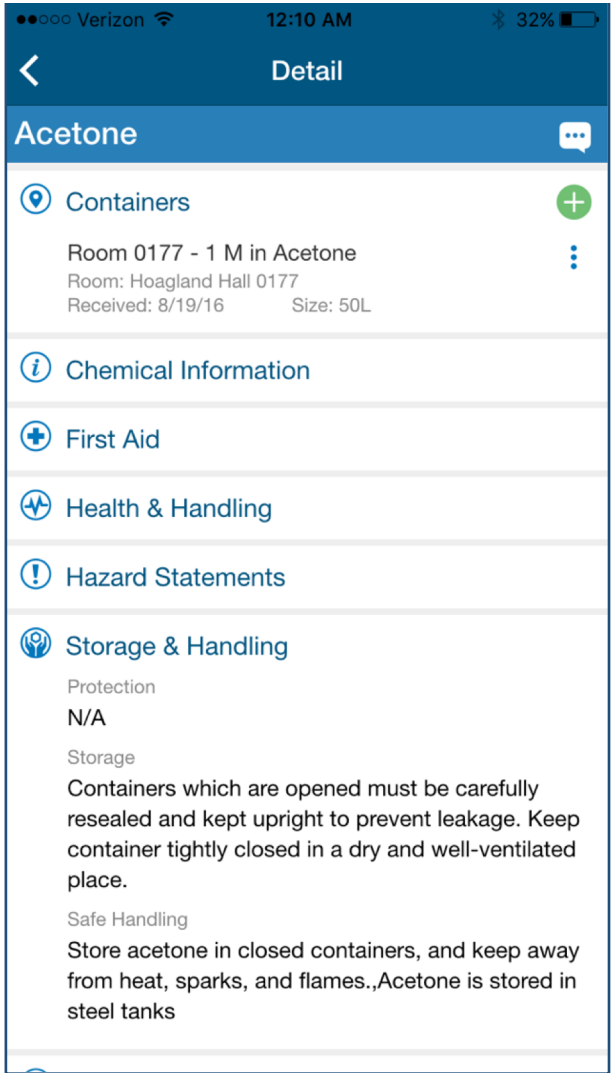
- incorporate best practices for chemical data, green chemistry, and risk assessment methodologies
- facilitate application of authoritative chemical safety data to decision making at the laboratory scale
- develop reports for clear communication and use by students, instructors, lab managers and safety personnel
- test efficacy of visual indicators in existing chemical safety lesson plans and different classrooms
- organic chemistry teaching laboratory use case as well-defined, widespread and a key entry point for chemistry majors into process design and evaluation

Mobile Management Tool

UC Chemicals

University of California chemical inventory





Information Ground Rules

- Information tools do **not** make safety decisions or recommendations
  - tools can help organize and present authoritative data in useful ways based on expert methodology to help facilitate decision making in risk assessment and safety planning
- Data sources and tools for using information are *not necessarily* (or even usually) the same system
  - most sources of chemical safety data are government agencies or chemical suppliers that can be referenced in systems tailored to manage the data specific to the needs of different audiences, for example laboratory students
- Information is only as good as source data and their curation
  - provenance is critical
  - accurate reporting and interoperability is critical

FAIR principles help us exchange data, accurately

- Findability – unique safety angle, safety info generated down the hall is not necessarily findable
- Accessibility – safety info needs to be free/open, not to conflate with IP
- Interoperability
  - good metadata - provenance - the difference b/w fake news and science
  - this is the key one – [point to Carmen's experience and need to share lessons learned - and provenance for critical evaluation]
- Re-usable (text-locking issue, different units/methods, etc.)

Information system layer cake

- **INTERFACE**
  frosting
- **FUNCTIONALITY**
  yummy cake
- STRUCTURE
  leavening
- DATA
  ingredients

Building a RAMP layer cake

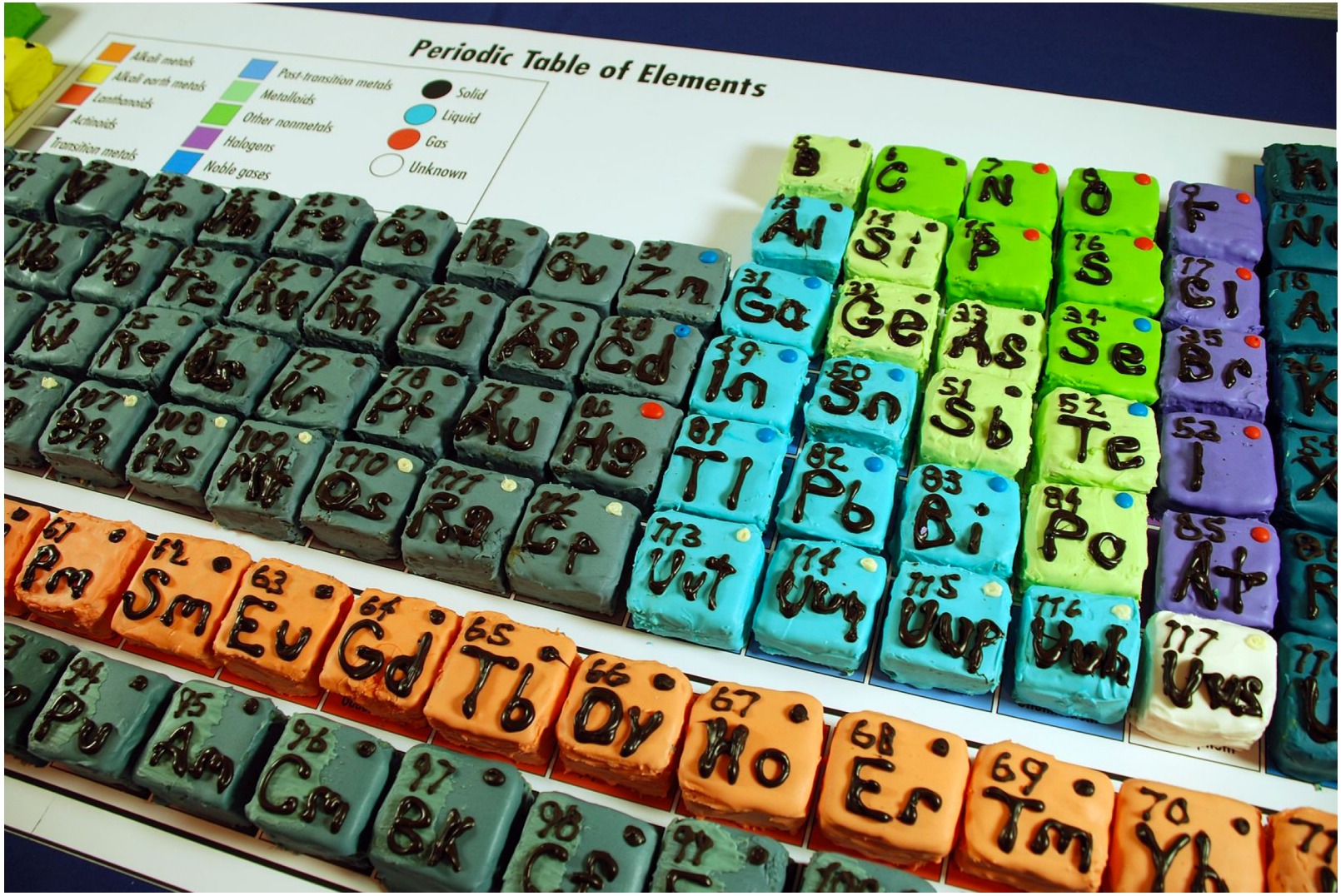
0. Source raw ingredients = **public safety data warehouse (*NLM*)**
1. Recipe ingredients = **Laboratory Chemical Safety Summary (LCSS)**
2. Measure portions = **extract needed data from LCSS**
3. Mix ingredients = **incorporate data into RAMP template**
4. Bake = **risk analysis (method from *Hazard Assessment*)**
5. Eat = **apply to experimental planning, safety controls, emergency procedures**
6. Clean up = **waste disposal**
7. Make notes on your fabulous recipe & share with friends = **document your risk assessment and contribute to lessons learned**

Search & Retrieve

Data curation

RAMP process

RCRA
Control banding
Publications
CSL



INTERNATIONAL YEAR OF THE PERIODIC TABLE 2019