# Introducing a Safety Guidance Chapter in the Fourth Edition of the ACS Style Guide

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CONNECTING CHEMISTRY AND SAFETY

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# Chemistry Professionals

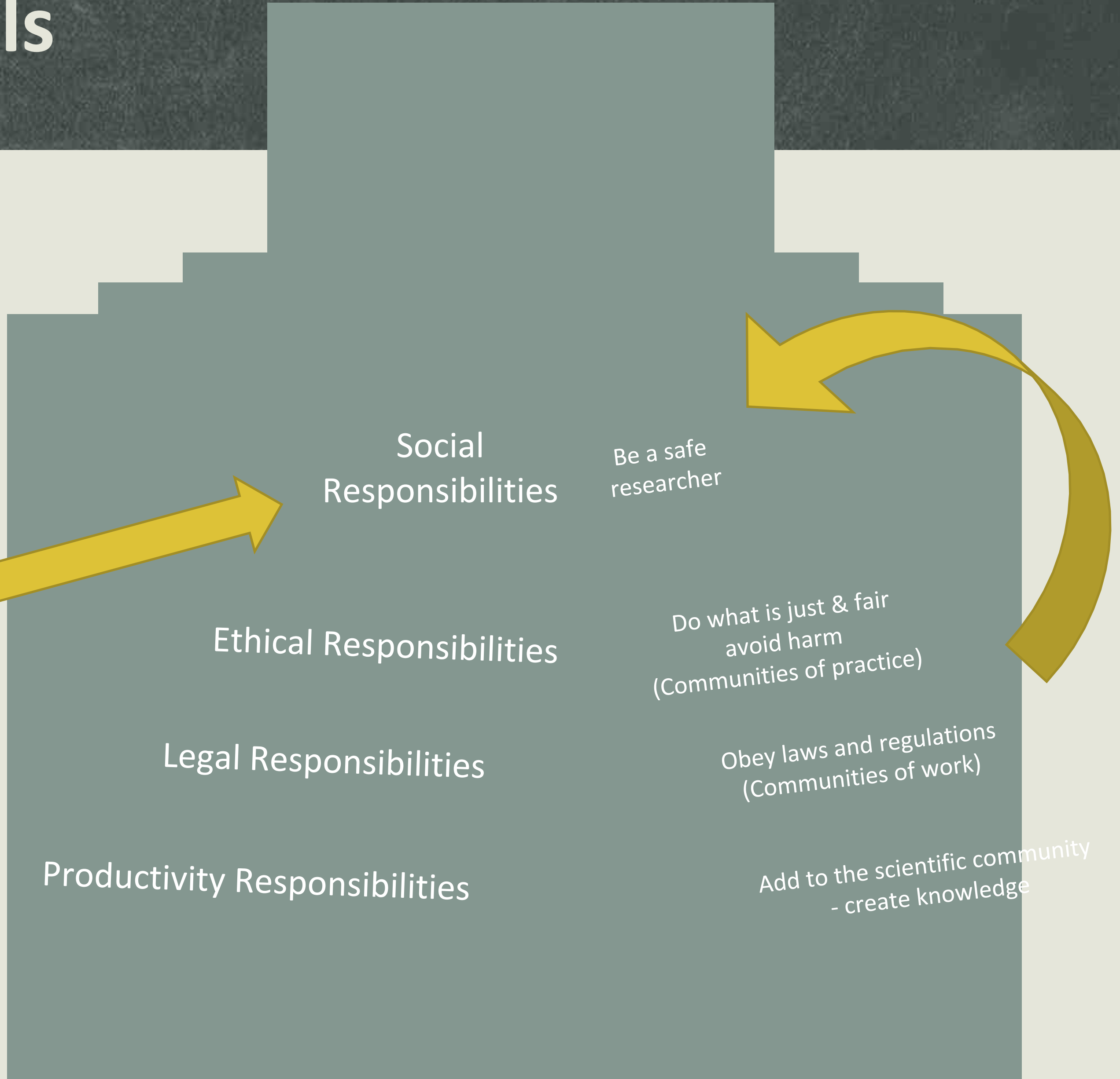
***Chemistry professionals have ethical and legal responsibility to work with chemicals safely.***

*They protect themselves, their communities, and the wider environment from the risks associated with the hazards of chemicals.*

*They address safety and health issues when contributing to the scientific literature.*

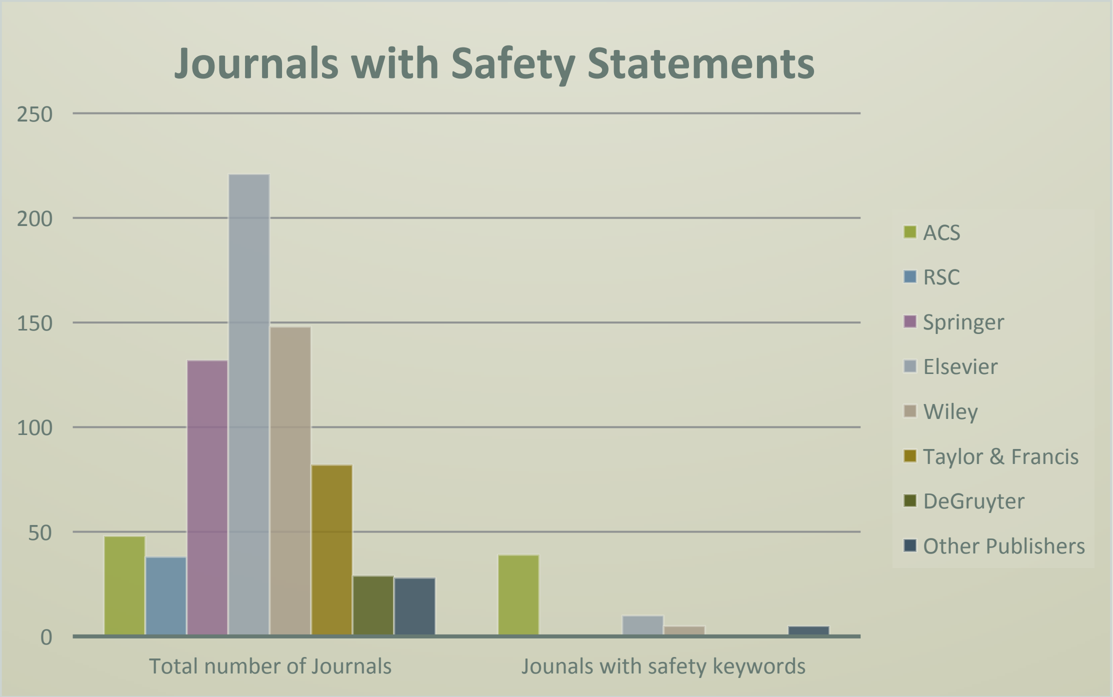
***Chemistry professionals need to develop competency in evaluating hazards, conducting assessments, and mitigating the risks of those hazards.***

https://www.acs.org/content/acs/en/chemical-safety/workplace-and-industry.html



In 2016, Grabowski and Goode examined 726 chemistry journals from 28 different publishers, to determine the nature of chemical safety precautions that authors were asked to include in manuscripts.

What they found was that **only 8% of the journals surveyed included any one of four keywords – caution, hazard, safety or danger in author guidelines**.



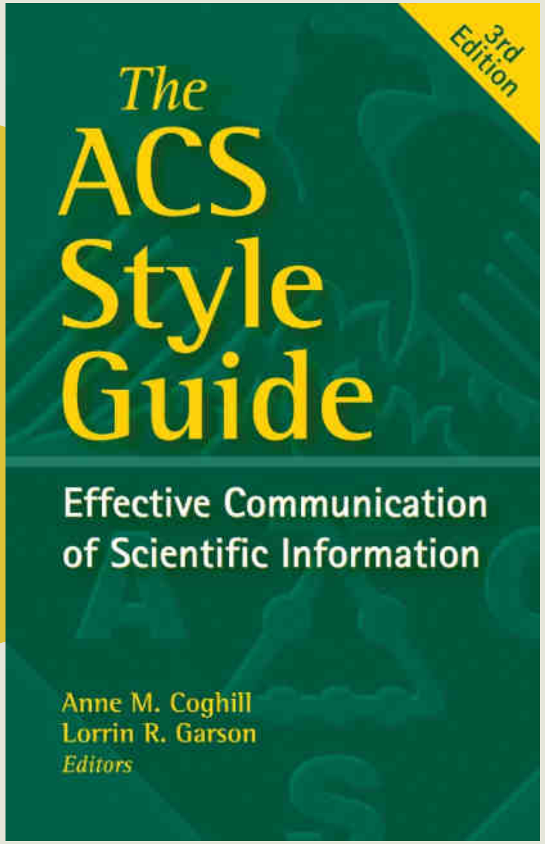

[1]Goode, S. R.; Grabowski. L. E. Review and analysis of safety policies of chemical journals. *J. Chem. Health Saf.* **2016,** *23*, 30-35. https://doi.org/10.1016/j.jchas.2015.10.001 (accessed Jan. 31, 2019).

# “Communicating Safety Information”

**016** – Grabowski and Goode examined hemistry journals to etermine the nature of chemical safety precautions.

**2017** – ACS Publications added a requirement in their journals for authors to include a safety statement in published work.

**2019** – The logical continuation of this effort is to provide the chemistry enterprise with guidance on developing and evaluating safety statements.

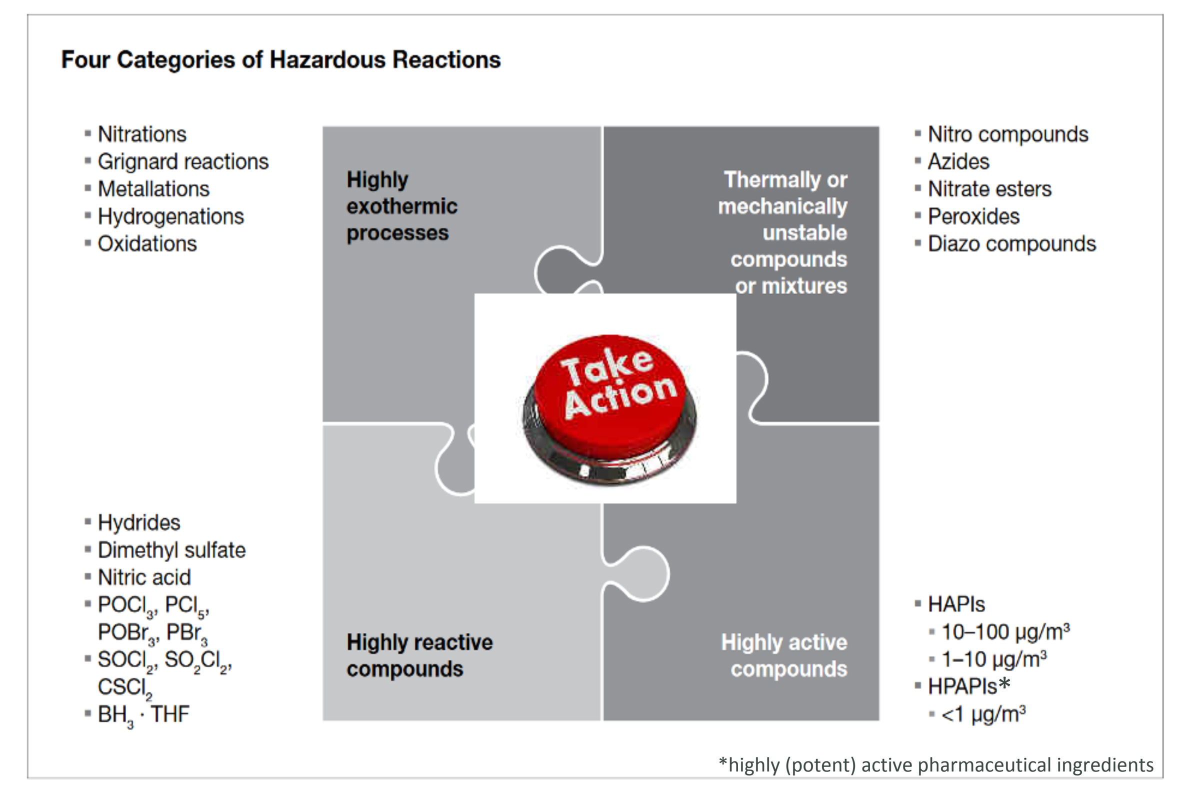



The fourth edition of *The ACS Style Guide* will include ***an all new chapter*** to provide authors with guidance on how to effectively communicate hazards and risks associated with published research.

# Safety Summaries

# Safety Guidelines in Scientific Publications - Goal

- The <u>**goal**</u> is to alert readers to unusual hazards or procedures which present significant risk or require special control measures beyond those reasonably anticipated to be commonly present in a chemistry teaching or research laboratory setting.
- It is expected that scientists *schooled in the art* and following published procedures will appropriately prepare for commonly known hazards in their field of study.




https://dottikon.com/dottikon-es-de/core-technologies/hazardous-reactions/

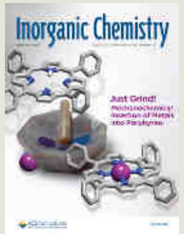
# Safety Guidelines in Scientific Publications…

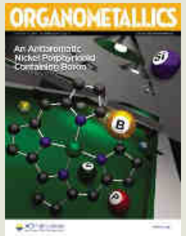
- …will help organize and communicate safety information specific to an experimental method in a consistent manner appropriate to manuscripts.
- …should inform readers about hazards requiring caution beyond common laboratory safety measures.
- …are intended to help those reproducing experiments to understand, mitigate, and prepare for unusual or special risks in reported methods.

# Safety information included in scientific publications is subject to the professional judgment of authors, editors and reviewers and will necessarily vary depending on the…

- J. Org. Chem.


- Inorg. Chem. & Organometallic




- J. Chem. Educ.

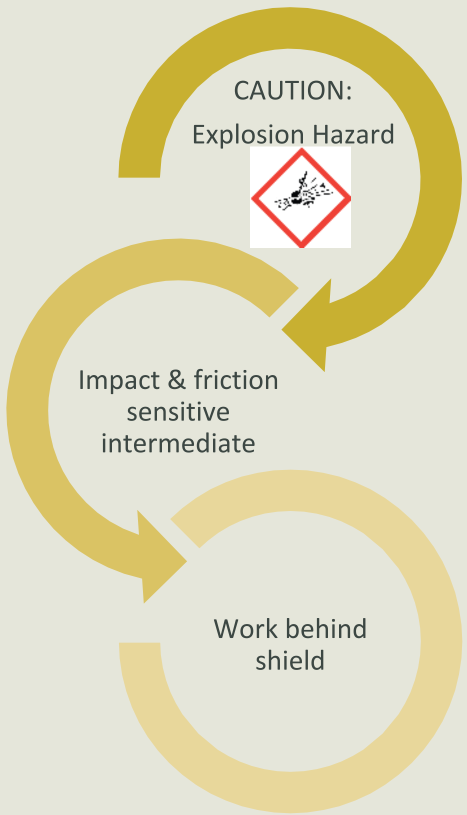

***…journal***

the ***chemistry***

& the ***audience***

# Communicating Experimental Hazard

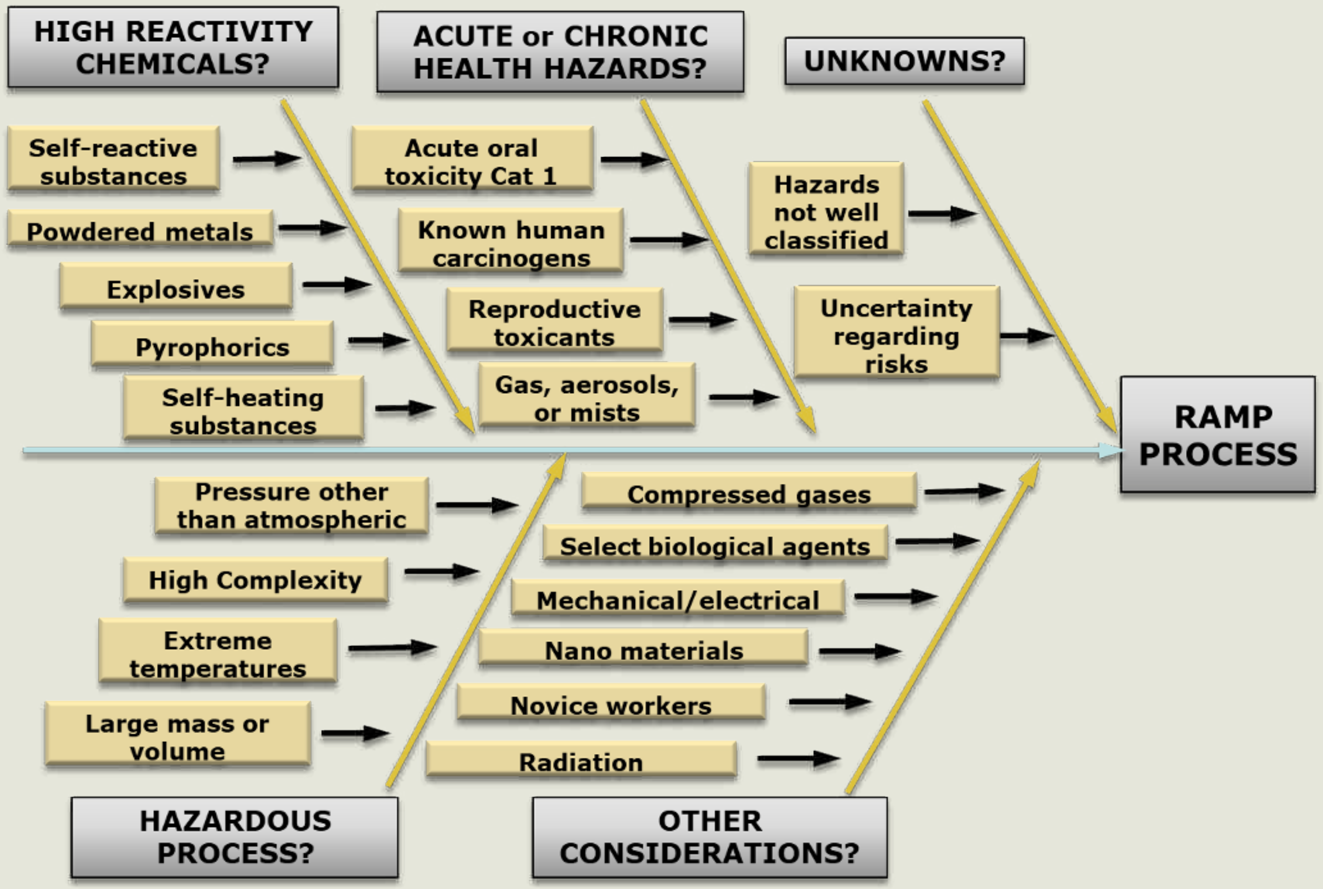
- The safety summary statement describing significant hazards of concern should be a precise communication of hazard management from the author regarding the specific experimental scenario directed to researchers and others downstream reproducing the science.
- In most cases the safety summary statement would be included in proximity to the experimental procedures or methodology sections, though in some cases hazards noted in observation may be indicated by footnotes.
- The information in a statement should be based on the assessed risks of the experimental processes.



# Determining Experimental Hazard


- We know that experimental hazards can result from a variety of agents, conditions, and/or activities.
- The information in a safety summary should address any type of hazard presenting significant risk based on assessment, be it due to the chemicals involved, the science involved, the equipment involved, or the environment where the work is being performed.

# Researching Risk Assessment

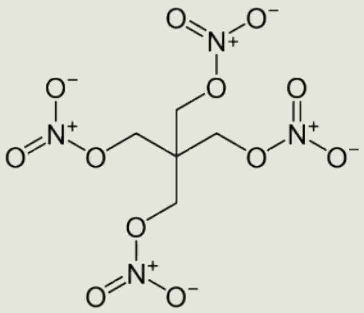



- **Recognize hazards** – Using available information from chemical labels, SDSs, documented procedures, experiential knowledge.
- **Assess risk** – Evaluate the hazards and potential for unwanted events using authoritative chemical properties and safety information.
- **Minimize risk** – Implement hazard prevention and risk management strategies into operating procedures.
- **Prepare for Emergencies** – Plan for contingencies to mitigate the effects of any exposure or damage that could occur.

# Communicate the Risk from High Hazard Chemicals Using GHS

| GHS Symbol | Hazard Class | Hazard Description |
|---|---|---|
|  | Explosive | Substances (Div. 1.1, Div. 1.2, Div. 1.3) which have an explosion hazard, whether mass or projection. (H201,H202, H203) |
| | Self-Reactive | Substances (Type A, B, or C) which can detonate, deflagrate, or self-heat under storage or handling conditions. (H240, H241, H242) |
|  | Flammable | Category 1 substances (gases, aerosols, liquids, or solids) which are readily ignitable under the reaction conditions. (H220, H222, H224, H228) |
| | Pyrophoric | Category 1 substances (liquids or solids) which ignite upon contact with air. (H250) |
| | Self-Heating | Category 1 substances which self-heat sufficiently to ignite. (H251) |
| | Organic Peroxide | Type A organic peroxides which, as stored or handled, can detonate or deflagrate rapidly. (H240) |
|  | Acute Toxicity | Category 1 substances. Concentration varies in this category based on the route of entry. $LD_{50} \leq 50$ mg/kg bodyweight (dermal) or $LC_{50} \leq 100$ ppmV; ≤ 0.5 mg/L; ≤ 0.05 mg/L (inhalation of gases, vapors, dusts & mists - respectively) (H310, H330) |
|  | Respiratory Sensitizer | Category 1A substances which show a high frequency of occurrence for respiratory sensitization in humans based on testing and/or severity. (H334) |
|  | Germ Cell Mutagenicity | Category 1A substances which have positive evidence from human epidemiological studies. (H340) |
| | Carcinogenicity | Known to, or presumed to have carcinogenic potential for humans based on human (1A) or animal evidence (1B). (H350) |
| | Reproductive Toxicity | Known to, or presumed to be a human reproductive toxicant based on human (1A) or animal evidence (1B ). (H360) |
| | Specific Target Organ Toxicity (STOT), Single Exposure | Category 1 substances that have produced significant toxicity in humans based on reliable human or animal evidence. (H370) |

# Specifically Consider Hazards from All Sources

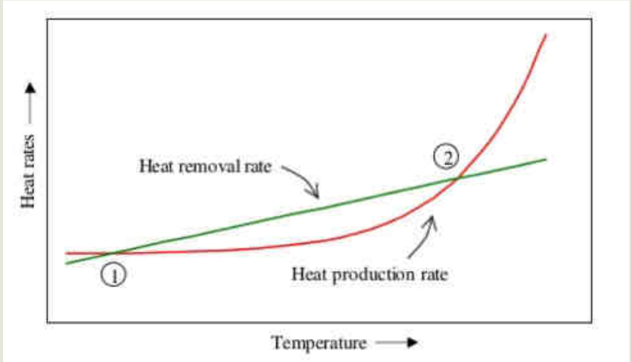



$(N_{Carbon} + N_{Oxygen}) / N_{Nitrogen} \geq 3$

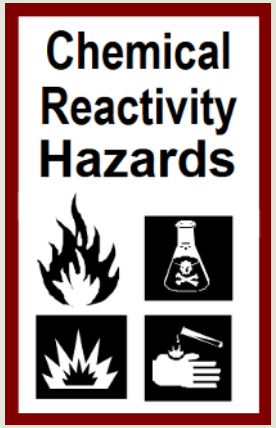
https://ehs.stanford.edu/reference/information-azide-compounds



- Elevated pressure or temperature where apparatus or conditions could reasonably lead to a fire, explosion, or loss of containment
- Oxygen at greater than 25% or oxygen/fuel mixtures which are ignitable
- Compounds with a C:N ratio less than 5 carbons per nitrogen (e.g. pentaerythritol tetraazide)
- Oxidations of organic molecules, particularly at elevated temperature and/or gram scale or greater
- Processes with high exothermicity that could lead to a run-away reaction
- Processes in which the energetics of scalability are insufficiently defined or require special cooling
- The addition of complexity (e.g., biological pathogens, radiation, nanoparticles, etc.) into the research




https://www.slideshare.net/BobvanWoezik/b-van-woezikrunaway-and-thermally-safe-operation-of-a-nitric-acid-oxidation-in-a-semibatch-reactor

# Assessing Risk in Local Context

Risk is the probability that a hazard will result in an adverse consequence, in any given situation:
**Risk Rating (RR) = Probability of Occurrence (OV) x Severity of Consequences Value (CV)**

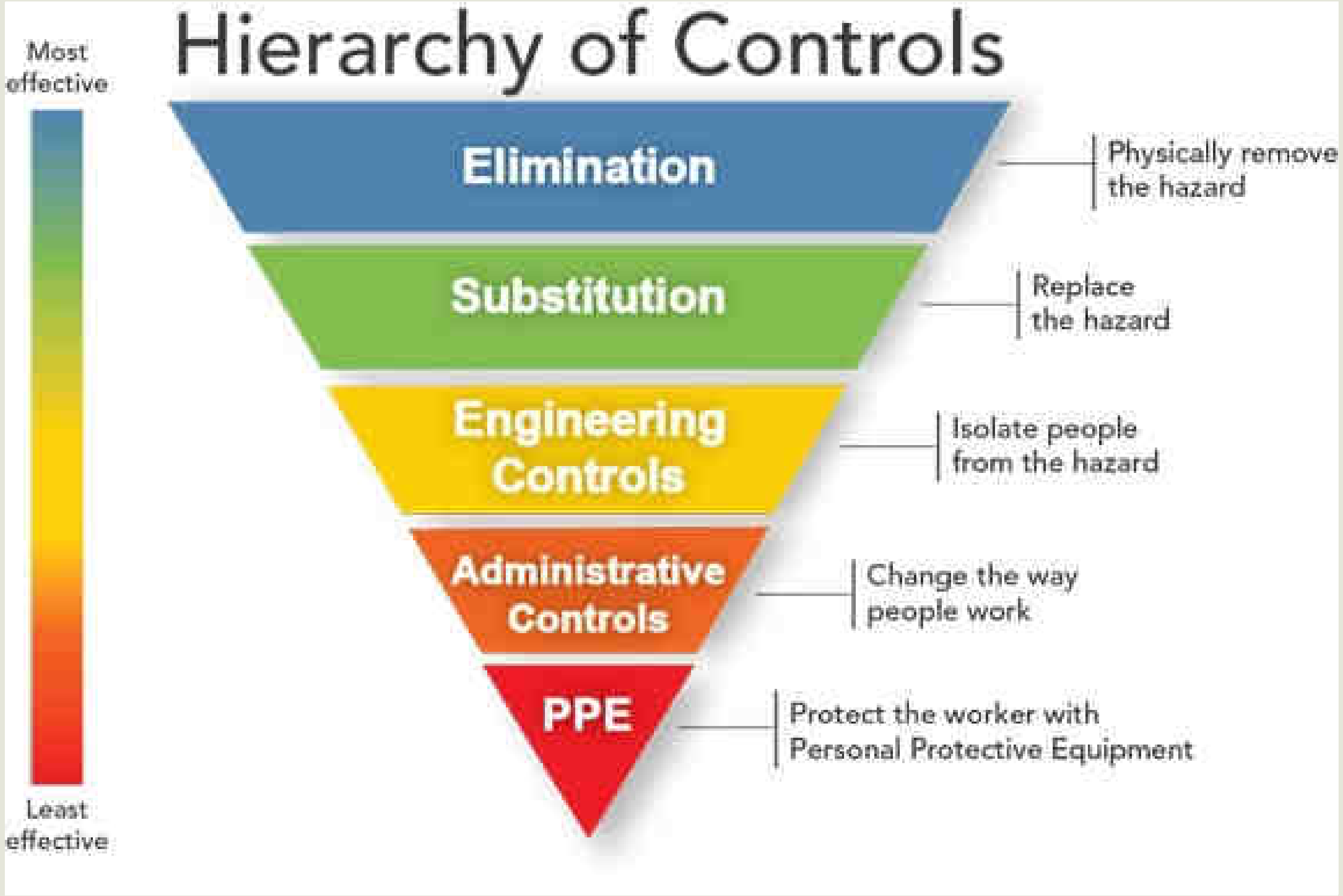
| | | Consequence | | | | |
|---|---|---|---|---|---|---|
| | | Insignificant | Minor | Moderate | Major | Severe |
| Likelihood | Almost certain | Medium | High | High | Extreme | Extreme |
| | Likely | Medium | Medium | High | Extreme | Extreme |
| | Possible | Low | Medium | Medium | High | Extreme |
| | Unlikely | Low | Low | Medium | High | High |
| | Rare | Low | Low | Low | Medium | High |

https://safety.unimelb.edu.au/incident-reporting/incident-reporting-risk-matrix

## Resources (sample):

- ACS Chemical and Laboratory Safety – acs.org/safety (*Safety in Academic Chemistry Laboratories, Identifying and Evaluating Hazards in Research Laboratories*)
- National Research Council – *Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards*
- National Library of Medicine, National Institutes of Health (*PubChem Laboratory Chemical Safety Summaries, ToxNet, Hazardous Substances Databank*)
- National Oceanic and Atmospheric Administration – *Computer-Aided Management of Emergency Operations* (CAMEO)
- Urben, P. G. *Bretherick's Handbook of Reactive Chemical Hazards*, 8th Edition (2017)

# Minimizing Risk




The National Institute for Occupational Safety and Health (NIOSH), https://www.cdc.gov/niosh/topics/hierarchy/default.html

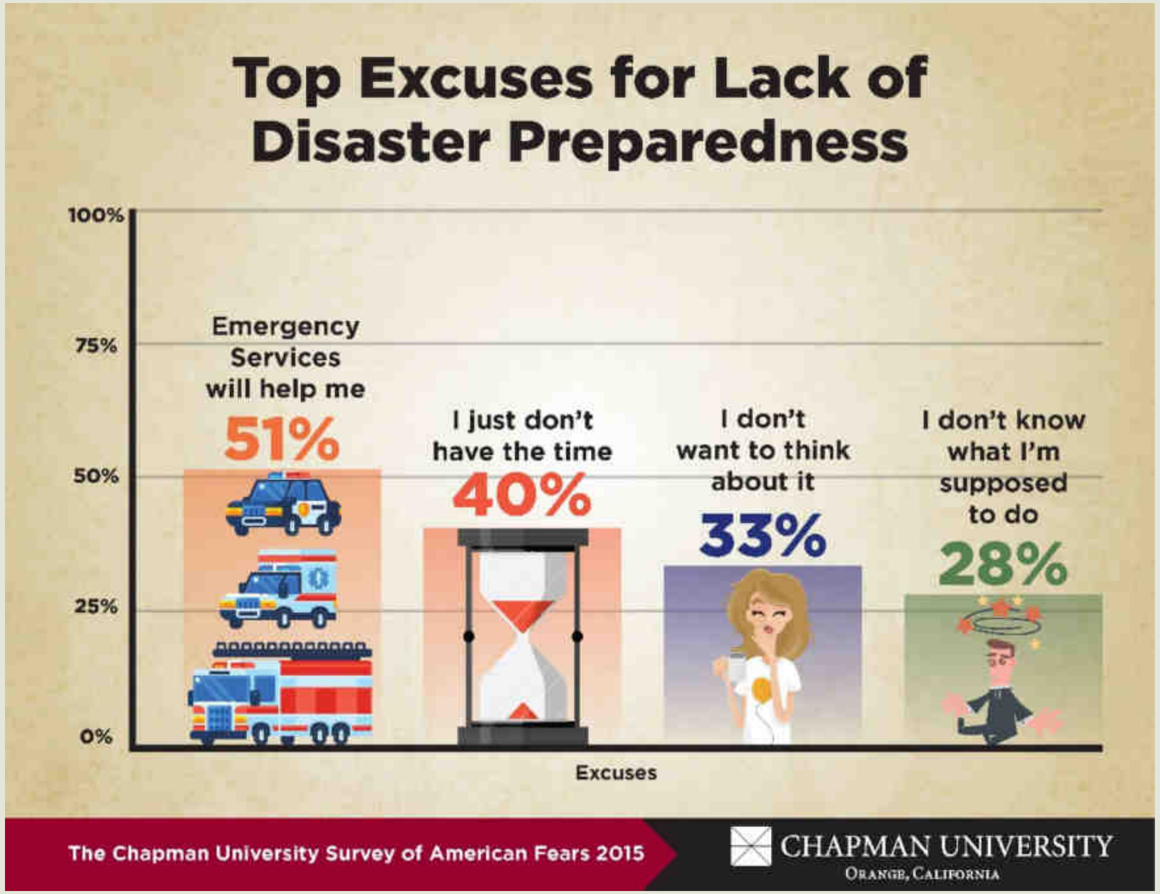
## EXAMPLE CONTROL STRATEGIES:

- **Eliminate**: different methodology (e.g., ball milling vs. solvent-based extraction)
- **Substitution:** less hazardous solvent (e.g., lower flammability, lower toxicity)
- **Engineering:** fume hood, correct equipment (e.g., cannula transfer)
- **Administrative:** regular lab procedures (e.g., SOPs)
- **PPE:** correct gloves (based on chemical resistance*)

* https://eta-safety.lbl.gov/doc/vwr-glove-chemical-resistance-chart

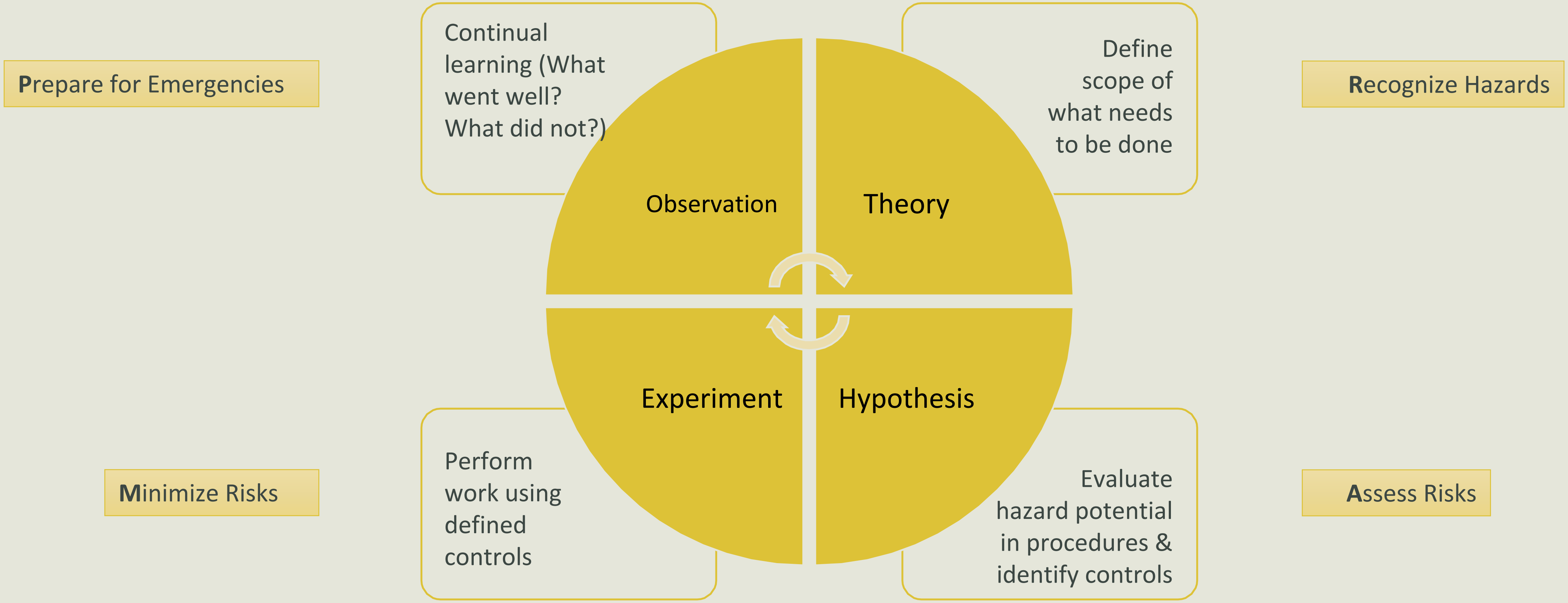
# Preparing for Emergencies

- A risk assessment process can help zero in on places in the procedure where loss of control could result in significant danger and what mitigation options could be most effective in reducing chance of harm.
- Preparing for the potential of emergencies can provide direction and focus for appropriate response should unanticipated circumstances arise.




https://www.chapman.edu/wilkinson/research-centers/babbie-center/survey-american-fears.aspx

# Integration of Hazard Identification, Evaluation, and Control with the Scientific Method




Adapted from: [Identifying and Evaluating Hazards in Research Laboratories]

# General Information Checklist – Safety Summary Statement

| | |
|---|---|
| √ | Names and CAS Registry Numbers of compounds and substances used or generated in the experiment that are of notable hazard, including products, intermediates, solvents, catalysts, etc. (e.g., substances in the categories listed in Table 1) |
| √ | GHS hazard communication elements for the hazardous compounds noted, including symbol, signal word, hazard statement, code and category, as provided by the manufacturer |
| √ | Note novel compounds, or closely related known analogs that have had incidents reported, and assume highest precaution based on active functional groups |
| √ | Note concentration of reagents and scale of the experiment for the specific procedure used (i.e., do you know the upper limits for scale of your specific procedure) |
| √ | Note experimental conditions and process parameters necessary to maintain control of the reaction with highly reactive materials (e.g., temperature or pressure control) |
| √ | Note laboratory equipment used to safely handle particularly hazardous compounds (e.g., cannula transfer procedure) |
| √ | Note appropriate mitigation strategies required beyond basic PPE (e.g., face shield, glove box) |
| √ | Note appropriate emergency equipment needed beyond standard laboratory equipment (e.g., metal fire suppressant) |
| √ | Note any modifications to equipment which could result in increased risk (e.g., electrical modifications) |
| √ | Note any additional laboratory or facility requirements (e.g., biohazardous or radioactive control laboratories) |

# Safety Summaries

Examples

# Examples - Research

“$TMSN_3$ was transferred from the commercial container to a pressure bomb excluding air and moisture. In laboratory scale, $TMSN_3$ was always handled in a ventilated enclosure (fume hood) to prevent exposure to $HN_3$ vapors. On kilogram scale, handling of $TMSN_3$ was done using double gloves (inner-nitrile surgical style, outer-silvershield), a silvershield apron, and a supplied air respirator.”

González-Bobes, F.; Kopp, N.; Li, L.; Deerberg, J.; Sharma, P.; Leung, S.; Davies, M.; Bush, J.; Hammand, J.; Hrytsak, M. Scale-up of Azide Chemistry: A Case Study. *Org. Process Res. Dev.* **2012,** *16,* 2055.

# Examples - Research

"Caution! tert-Butylithium 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. [Note added August 2009]."

Busacca, C. A.; Eriksson, M. C.; Haddad, N.; Han, S. H.; Lorenz, J. C.; Qu, B.; Zeng, X.; Senanayake, C. H. Practical Synthesis of Di-tert-Butyl-Phosphinoferrocene. *Org. Synth.* **2013**, *90*, 316-326. DOI: 10.15227/orgsyn.090.0316. http://www.orgsyn.org/demo.aspx?prep=v90p0316

# Example – Teaching Audience

- [hold for new flame test paper in JCE, good hazard statement….]
- [https://doi.org/10.1021/acs.jchemed.8b01010]

# Acknowledgements


- ACS Division of Chemical Health & Safety (CHAS)
  - Especially Harry Elston & Neal Langerman for initial supporting documentation
- ACS Committee on Chemical Safety (CCS)
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