Information Literacy in the Disinformation Era:

Challenges in working with chemical safety information

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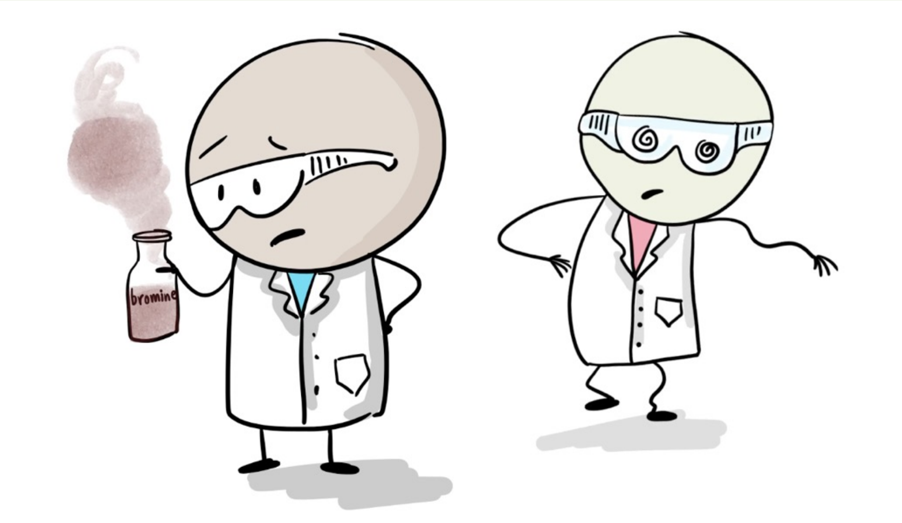


Information without context could be a safety issue…

What sort of PPE is appropriate when using DMSO, a water-miscible solvent commonly used in laboratories?

- Relatively low flammability
- Apparently low toxicity
- But… readily absorbed through skin

➢ *What if you have dissolved other toxic materials in DMSO?*

Sigma-Aldrich

www.sigmaaldrich.com

SAFETY DATA SHEET

Version 6.8
Revision Date 10/07/2020
Print Date 11/20/2020

1.1 Product identifiers

Product name : Dimethyl sulfoxide

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Rapidly absorbed through skin.

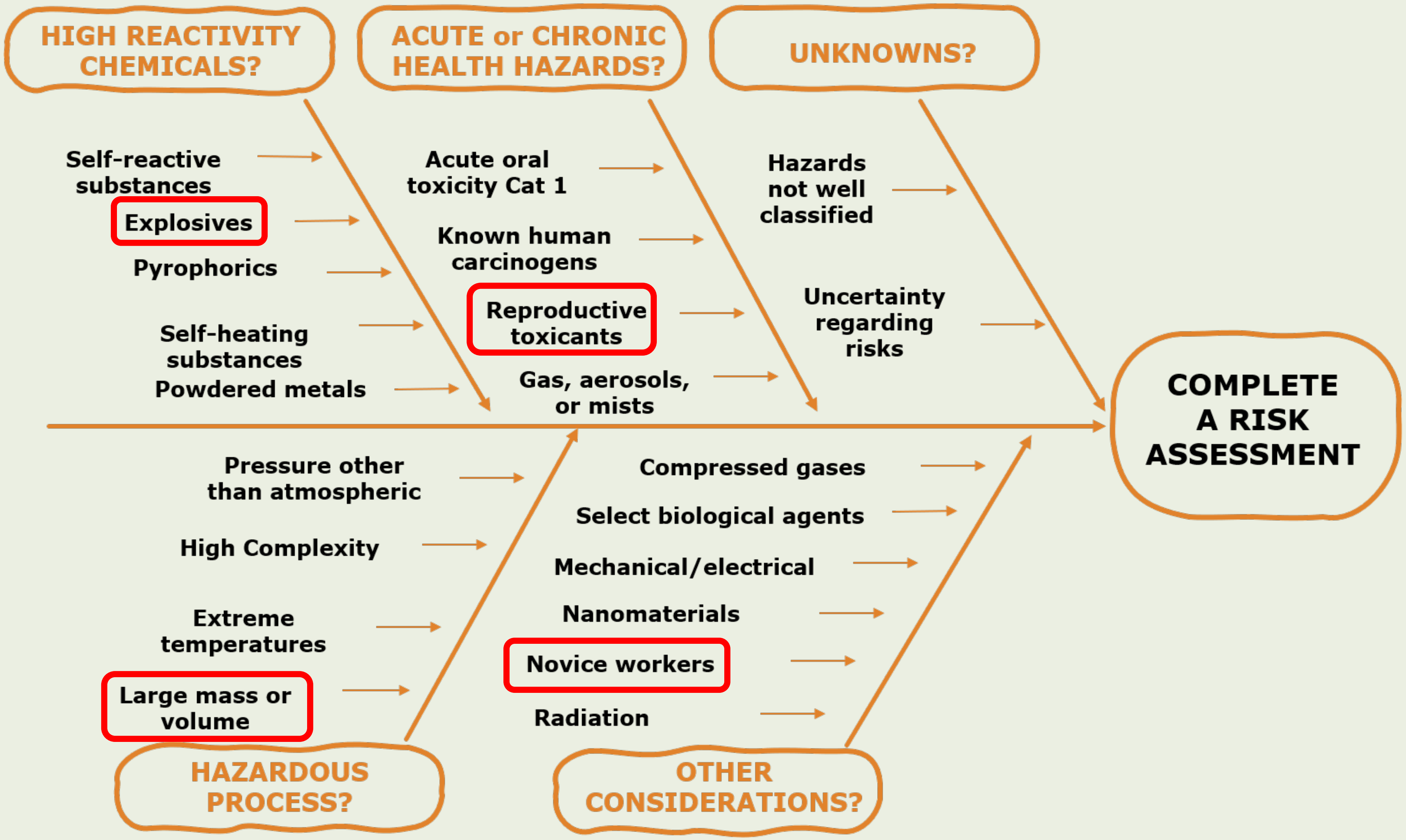
European Chemicals Agency (ECHA)

Irritant

Japan Chemical Management Center (NITE-CMC)

Health Hazard

Context is important in laboratory safety



RAMP: informed risk assessment

Recognizing hazards

Assessing risk

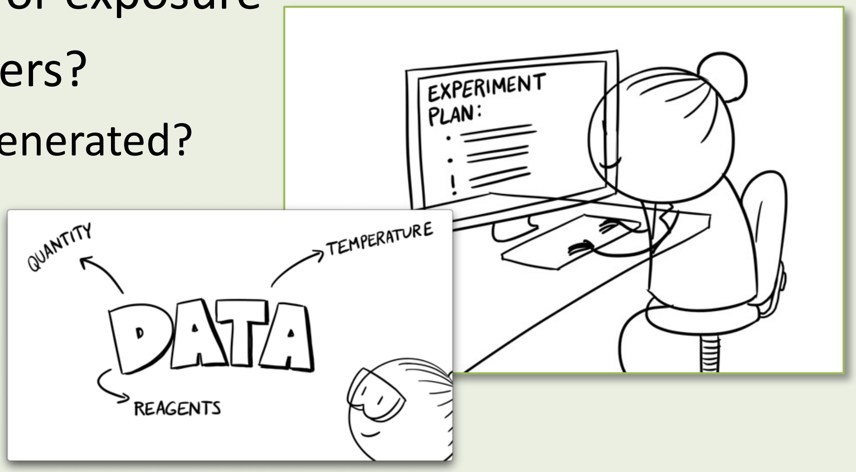
Minimizing risk

Preparing for emergencies

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

- What is the relative degree of hazard given scale, reactivity, toxicity?
- How likely could a hazardous event or exposure occur within experimental parameters?
  - Are flammable or noxious vapors generated?
  - Are there known incompatibilities between reagents?
  - Is the run temp. close to the flash point of any reagents?



Many sources of chemical safety information, could be wrong for context

Scientific information

- Chemical properties
- Methodology

“Practical”

- Procedural, protocols
- Equipment specifications

Legally defined

- Classifications
- Policies,
  reporting requirements

Key types of available data & information
for considering chemical safety & risk assessment

GHS classifications

Reactivity

Toxicity

Chemical & physical properties

Specialized equipment & procedures

Specialized PPE

Cautionary statements in published methods

Where to find it *(different than usual sources)*

Label and Safety Data Sheets (SDS) from manufacturer

GHS info compiled by national & international regulatory bodies

Safety data cards/sheets/lists from national & international agencies

Equipment guides from manufacturers

Safety guides from scientific bodies

Institutional EHS offices

Process research literature

Compiled references and databases from above sources

Factors

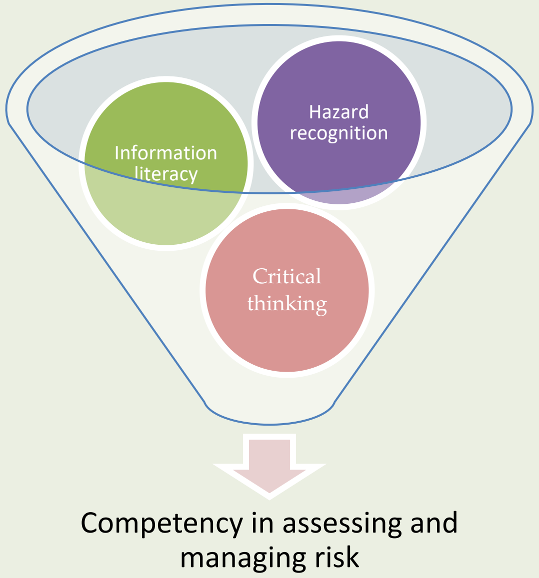
- Scale: research lab, industrial transport?
- Readers: emergency responder, researcher, student?
- Use of chemical: concentration, amount?

Safety information resources

Resource	Type	Audience	Sources cited?
SDS: Safety Data Sheets	Legal	Any user (generic)	
PubChem LCSS: Laboratory Chemical Safety Summaries	Scientific	Scientist (researcher)	✓
CAMEO: Computer-Aided Management of Emergency Operations	Practical	Emergency responder	✓

"It is vital in this era that students who will be working in our twenty-first-century research laboratories be taught how to assimilate useful and factual safety information into a competency" (Sigmann, 2018)

- Essential to support critical decision making around safety
- How to assess "useful" and "factual"?



DOI: 10.1016/j.jchas.2017.11.002

How to “read” an SDS

Chemical understanding needed:

- How concentration, amount, pressure & temperature can have a profound effect on reactions
- The elements of combustion (the fire tetrahedron) and how physical and chemical properties of solvents affect flammability
- Thermal runaway reactions (heat production vs. heat removal)
- Basic toxicology, including acute vs. chronic exposure, routes of entry, and testing methods
- Common groups of shock sensitive, self-heating, pyrophoric, oxidizing, and polymerizing chemicals
- The significance of the n-Octanol/Water Partition Coefficient

Navigating & assessing information:

- Familiarity with symbols, acronyms, terms
- “No Data Available” vs. “Not Applicable” or “Not Established”
- Conflicting data (check multiple sources)
- *Original data sources not often cited*

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Colour: colourless
b)	Odour	No data available
c)	Odour Threshold	No data available
d)	pH	< 1.0
e)	Melting point/freezing point	No data available
f)	Initial boiling point and boiling range	120.5 °C (248.9 °F) - lit.
g)	Flash point	No data available
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapour pressure	49 hPa (37 mmHg) at 50 °C (122 °F)
l)	Vapour density	No data available
m)	Relative density	1.413 g/cm3 at 20 °C (68 °F)
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

Section 9. Physical and Chemical Properties

Information on Basic Physical and Chemical Properties

Appearance: Clear, colorless to pale yellow or brown liquid
Odor: Acrid, pungent
Odor Threshold: 0.75 - 2.5 ppm
Molecular Weight: 63.01 g/mol (nitric acid)
Chemical Formula: HNO_3 (nitric acid)
pH: < 1
Freezing Point, Range: -20 - -31.7°C (-4 - -25°F)
Boiling Point, Range: 117 - 120°C (243 - 248°F)
Evaporation Rate: -1 (BuAc = 1)
Flammability (solid, gas): Not applicable
Flash Point: Not applicable
Autoignition Temperature: Not applicable
Decomposition Temperature: 110°C (230°F)
Lower Explosive Limit (LEL): Not applicable
Upper Explosive Limit (UEL): Not applicable
Vapor Pressure: 9 - 10 mm Hg at 25°C (70°F)
Vapor Density: >1 (Air= 1)
Relative Density: 1.3551 - 1.4078 g/mL (11.31 - 11.75 lb/gal)
Viscosity: 2.0 - 2.2 cps
Solubility in Water: Complete
Partition Coefficient: n-octonal/water: Log Pow= -2.3
Volatiles by Volume (at 70°F): 100%

SDS excerpt (left) where the data was not carefully considered by the preparer.
Sigmann (2018). DOI: 10.1016/j.jchas.2017.11.002

National Library of Medicine
National Center for Biotechnology Information

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pubchem.ncbi.nlm.nih.gov/compound/Sodium-azide

COMPOUND SUMMARY

Sodium azide

Cite Download

PubChem CID	33557
Structure	 2D Find Similar Structures
Chemical Safety	 Acute Toxic, Environmental Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	N_3Na or NaN_3
Synonyms	sodium azide 26628-22-8 Azide, sodium Natriumazid Sodiumazide More...
Molecular Weight	65.01 g/mol

CONTENTS

- TOXNET
  - ChemIDplus
  - Hazardous Substances Data Bank (HSDB)
- CAMEO Chemicals
- CAS Common Chemistry
- EPA Chemicals under the TSCA
- EPA DSSTox
- EU REGULATION (EC) No 1272/2008
- European Chemicals Agency (ECHA)
- Hazardous Chemical Information System (HCIS), Safe Work Australia
- ILO International Chemical Safety Cards (ICSC)
- NITE-CMC
- NJDOH RTK Hazardous Substance List
- Occupational Safety and Health Administration (OSHA)
- Pistoia Alliance Chemical Safety Library
- PubChem
- The National Institute for Occupational Safety and Health (NIOSH)
- Wikipedia

PubChem Hydrazoic acid (Compound LCSS)

1 GHS Classification

Pictogram(s)	
Signal	Danger
GHS Hazard Statements	H200: Unstable Explosive [Danger Explosives] H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation] H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation] H370: Causes damage to organs [Danger Specific target organ toxicity, single exposure]
Precautionary Statement Codes	P201, P202, P260, P261, P264, P270, P271, P280, P281, P304+P340, P305+P351+P338, P307+P311, P312, P321, P337+P313, P372, P373, P380, P401, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

NITE-CMC

Source: NITE-CMC

Record Name: Hydrogen azide - FY2009

URL: https://www.nite.go.jp/chem/english/ghs/09-mhlw-0250e.html

Description: The chemical classification in this section was conducted by the Chemical Management Center (CMC) of Japan National Institute of Technology and Evaluation (NITE) in accordance with GHS Classification Guidance for the Japanese Government, and is intended to provide a reference for preparing GHS labelling and SDS for users.

Rationale for the classification
The substance contains chemical groups (adjacent nitrogen atom) associated with explosive properties present in the molecules. Pure substance can be judged to be "Unstable explosive" from the literature such as "Extremely explosive" (Sax (11th, 2004), PATTY (5th, 2001)), "Violently explosive" (Bretherick (7th, 2007)) and the information of "Extremely explosive and explode due to heating or in presence of glass shards, even without shocks." (Encyclopedia Dictionary of Chemistry (1994, the 3rd. impression)). Commercially available substance is the product diluted with solvents and is considered not to be "Explosives".
Based on a report that vapour exposure can irritate the eyes as an acute effect on human (ACGIH Sodium Azide (2001)), the substance was classified into Category 2.
Hydrazoic acid vapour is released from solutions of sodium azide, and the acid and salt moieties have the same degree of acute toxicity. There is a report that inhalation or congestion of sodium azide by humans can cause various symptoms (dizziness, blurred vision, dyspnea, tachypnea, hypotension, tachycardia, acidosis, and spasms), a paralyzed respiratory center, and can affect the cardiovascular system. Additionally, there is a report that azide is a direct-acting vasodilator (ACGIH Sodium Azide (2001)). Based on all information, the substance was classified into Category 1 (central nervous system, cardiovascular system). In addition, based on a report that exposure to hydrazoic acid vapours caused bronchitis (ACGIH Sodium Azide (2001)), the substance was classified into Category 3 (respiratory tract irritation).

cameochemicals.noaa.gov

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MyChemicals Collection

1.	SODIUM AZIDE	Remove
2.	SULFURYL CHLORIDE	Remove
3.	ACETONITRILE	Remove
4.	ETHYL ACETATE	
5.	HYDROCHLORIC ACID, SOLUTION	

Add Water | Add Reactive Group | Sort

Accidentally removed a chemical? Retrieve it h

Use the MyChemicals Collection to...

- View **chemical datasheets** (with respo on the name of any substance in the list
- Consider the **reactivity predictions** if t chemical's reactive hazards (including ai chemical datasheet.)
- Generate a **report** (with reactivity predi

Print Report

	SODIUM AZIDE	SULFURYL CHLORIDE	ACETONITRILE	ETHYL ACETATE	HYDROCHLORIC ACID, SOLUTION
SULFURYL CHLORIDE	**Incompatible** Explosive Generates gas Intense or explosive reaction Toxic				
ACETONITRILE	**Caution** Flammable	**Compatible**			
ETHYL ACETATE	**Caution**	**Incompatible** Generates gas Generates heat Toxic	**Compatible**		
HYDROCHLORIC ACID, SOLUTION	**Incompatible** Explosive Flammable Generates gas Generates heat Toxic	**Incompatible** Corrosive Generates gas Generates heat Intense or explosive reaction Toxic Unstable when heated	**Incompatible** Flammable Generates gas Toxic	**Incompatible** Corrosive Flammable Generates gas Generates heat Intense or explosive reaction	
WATER	**Incompatible** Generates gas Generates heat	**Incompatible** Corrosive Generates gas Generates heat Intense or explosive reaction Toxic	**Caution** Flammable Generates gas Toxic	**Caution** Corrosive Generates gas	**Caution** Corrosive Generates gas Generates heat

Hazards

What is this information?

The Hazard fields include special hazard alerts air and water reactions, fire hazards, health hazards, a reactivity profile, and details about reactive groups assignments and potentially incompatible absorbents. The information in CAMEO Chemicals comes from a variety of data sources.

Chemical Datasheet for **SULFURYL CHLORIDE**

Reactivity Alerts

- Water-Reactive
- Air-Reactive

Air & Water Reactions

Fumes in air. Reacts with moist air to give strongly acidic mists that are heavier than air. Decomposes slowly in water to give hydrochloric acid and sulfuric acid [Handling Chemicals Safely p. 881 1980]. Based on a scenario where the chemical is spilled into an excess of water (at least 5 fold excess of water), half of the maximum theoretical yield of Hydrogen Chloride gas will be created in 8.7 minutes. Experimental details are in the following: "Development of the Table of Initial Isolation and Protective Distances for the 2008 Emergency Response Guidebook", ANL/DIS-09-2, D.F. Brown, H.M. Hartmann, W.A. Freeman, and W.D. Haney, Argonne National Laboratory, Argonne, Illinois, June 2009.

Fire Hazard

Behavior in Fire: Toxic and irritating gases are generated. (USCG, 1999)

Health Hazard

Vapors cause severe irritation of eyes and respiratory system. Liquid burns eyes and skin. If ingested, can cause severe burns of mouth and stomach. (USCG, 1999)

Reactivity Profile

SULFURYL CHLORIDE reacts exothermically with water. Incompatible with strong oxidizing agents, alcohols, amines. Reacts violently with bases. Attacks many metals. Can react explosively with lead dioxide [Mellor 10:676 1946-47]. May react vigorously or explosively if mixed with diisopropyl ether or other ethers in the presence of trace amounts of metal salts [J. Haz. Mat., 1981, 4, 291].

Belongs to the Following Reactive Group(s)

- Acyl Halides, Sulfonyl Halides, and Chloroformates

Potentially Incompatible Absorbents

Use caution: Liquids with this reactive group classification have been known to react with the absorbents listed below. More info about absorbents, including situations to watch out for...

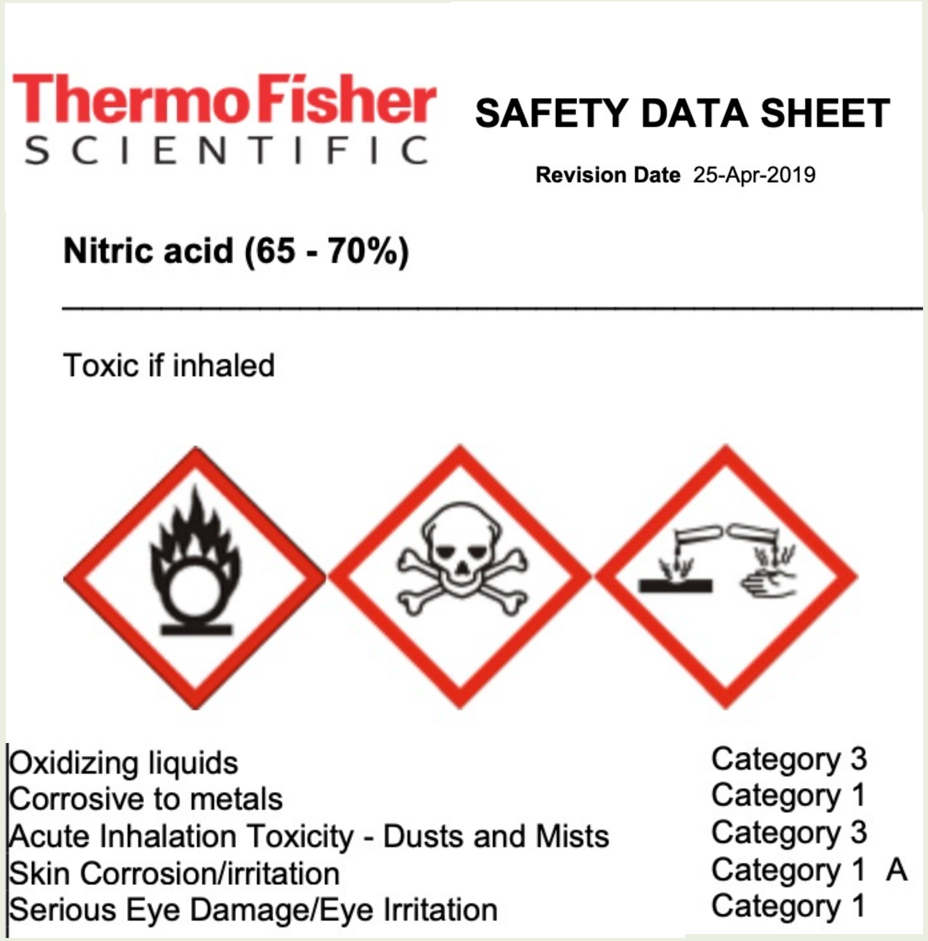
- Cellulose-Based Absorbents
- Mineral-Based & Clay-Based Absorbents
- Dirt/Earth

Assessment is ongoing

- Experiments & procedures change
  - Different solvents
  - Scale-up
  - Change in temperature, pressure, equipment
- Data quality & accessibility evolving
  - Assuming continuing access to public information, more safety data exchange
  - Greater availability of templates, tools, instruction
- Increasing complexity of research
  - Intra/interdisciplinary
  - High turn-over of personnel
  - International collaborations (linguistic, cultural distinctions)
  - Novel materials
  - Early students training programs

Exposure Control/PPE in different contexts

- ECHA SDS guidance (EU):
  *“The type of gloves to be worn when handling the substance or mixture shall be clearly specified based on the **hazard of the substance or mixture** and **potential for contact** and with regard to the **amount and duration of dermal exposure…**”*
- Questions to ask:
  - What chemicals will you be using, what chemical groups do these belong to?
  - Will you need to immerse your hands? Or just protect against potential splash?
  - Do you anticipate wearing gloves for hours (long/repeated procedure) or just a short task?
- Does the safety information indicate:
  - Glove material
  - Thickness
  - Breakthrough/penetration times


ThermoFisher SCIENTIFIC

SAFETY DATA SHEET

Revision Date 25-Apr-2019

Nitric acid (65 - 70%)

Toxic if inhaled

Oxidizing liquids	Category 3
Corrosive to metals	Category 1
Acute Inhalation Toxicity - Dusts and Mists	Category 3
Skin Corrosion/irritation	Category 1 A
Serious Eye Damage/Eye Irritation	Category 1

Section 8. Exposure controls/personal protection

“Wear suitable gloves and eye/face protection.”

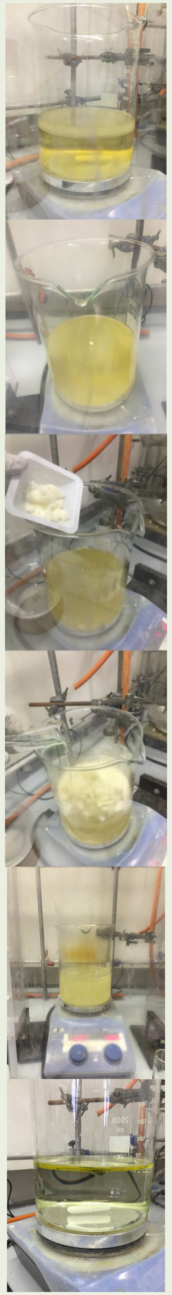
www.chemsafetypro.com/Topics/GHS/GHS_SDS_section_8_how_to_select_gloves_for_chemicals.html

Lab procedures should be “living documents”

- Written procedures should be fully re-assessed with any change to protocols, chemicals used, or lab setup
- Changes in one step of a procedure may have effects on the efficacy and safety of further steps
- Students in particular following steps as written may not be aware of the potential misalignment if something was changed but not re-assessed
- Always prudent to assess hazards and potential risk step by step for each job at hand (”Job Hazard Analysis”), even if you’ve done it before, change happens

Chemicals used did not match the current waste protocol

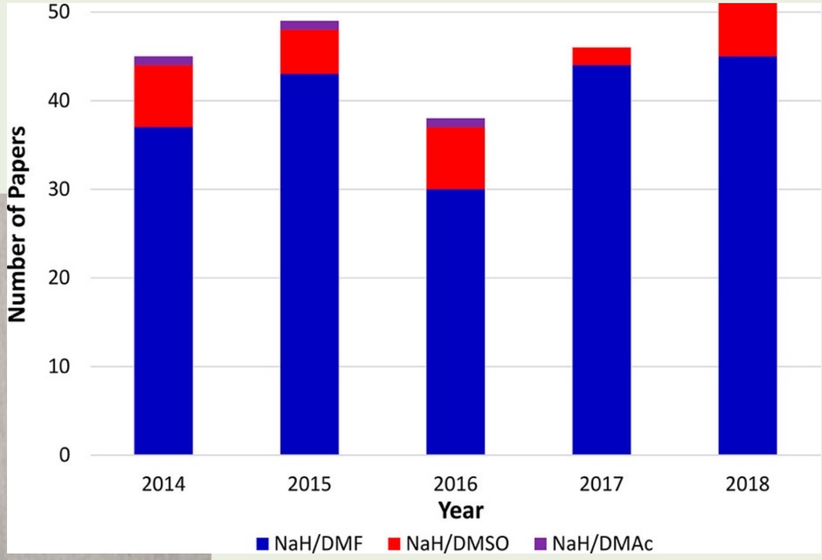
- Scenario 1
  - Procedure changed in practice but not in writing
  - Incompatible chemicals mixed in waste container resulting in explosion
  - Students did not know to assess the procedure for potential errors or hazards
- Scenario 2
  - Using procedure cited in literature that generates a ”mother liquor”
  - Likely still contains reactive reagents and users may not be authorized to treat waste
  - Neutralize known reagents as part of experimental procedure



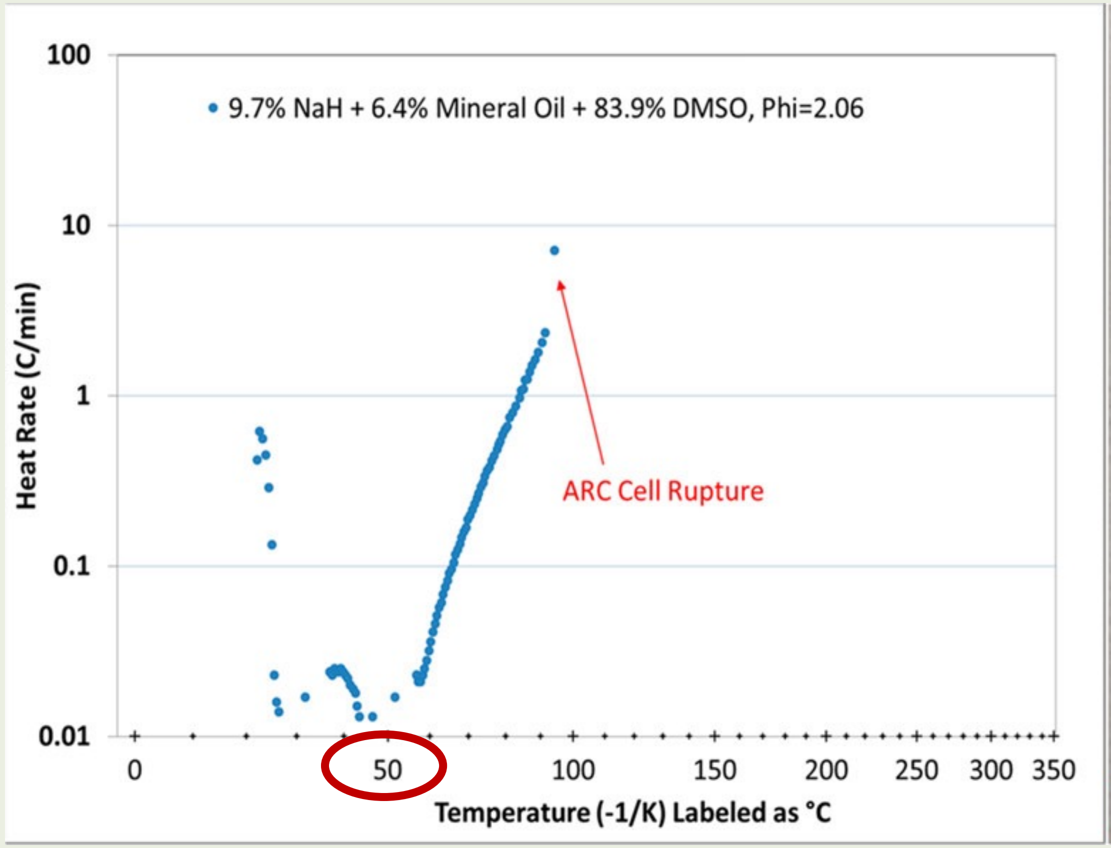
https://www.depts.ttu.edu/ehs/about/safety@ttu/lessons-learned/feb-2015.php

DOI: 10.1021/acs.joc.8b00270

Context of other chemicals



Portion of papers published in ***Organic Letters*** using these base/solvent combinations.



Accelerating rate calorimetry (ARC) heat rate profile of a NaH/DMSO mixture

"The data outlined in this contribution confirm that these reactive mixtures undergo exothermic decomposition at relatively low temperatures, occurring concurrently with the generation of noncondensable gases." (noxious, dimethyl sulfide)

DOI: 10.1021/acs.oprd.9b00276

Hazards of novel compounds…

Publication of a seminal paper on an "efficient, inexpensive, shelf-stable diazotransfer reagent"

- *Org. Lett.* 2007, **9**, 19, 3797–3800. DOI: 10.1021/ol701581g (**420 citations**)

2007

Correction: number of safety issues with preparation, storage and use, including explosion

- *Org. Lett*. 2011, **13**, 9, 2514. DOI: 10.1021/ol2007555 (**34 citations**)

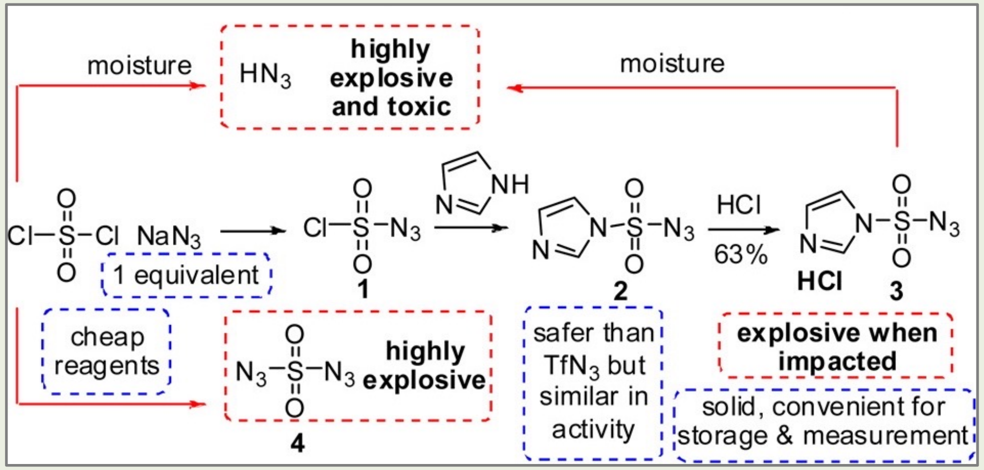
2011

Further publication on sensitivities of various other salts of diazo reagent, some more stable

- *J. Org. Chem.* 2012, **77**, 4, 1760–1764. DOI: 10.1021/jo202264r (**73 citations**)

2012

- Additional studies of sensitivities, new synthetic routes, more stable alternatives, etc.
- Awareness of this issue has advanced science and science safety
- It is important to conduct informed risk assessment of your work and to communicate useful information back to the community



Org. Lett. 2013, 15, 1, 18–21.
DOI: 10.1021/ol3028708

Not all diazo compounds are ~~hazardous…~~ *explosion hazards*

New safety statement requirements in scientific publications…

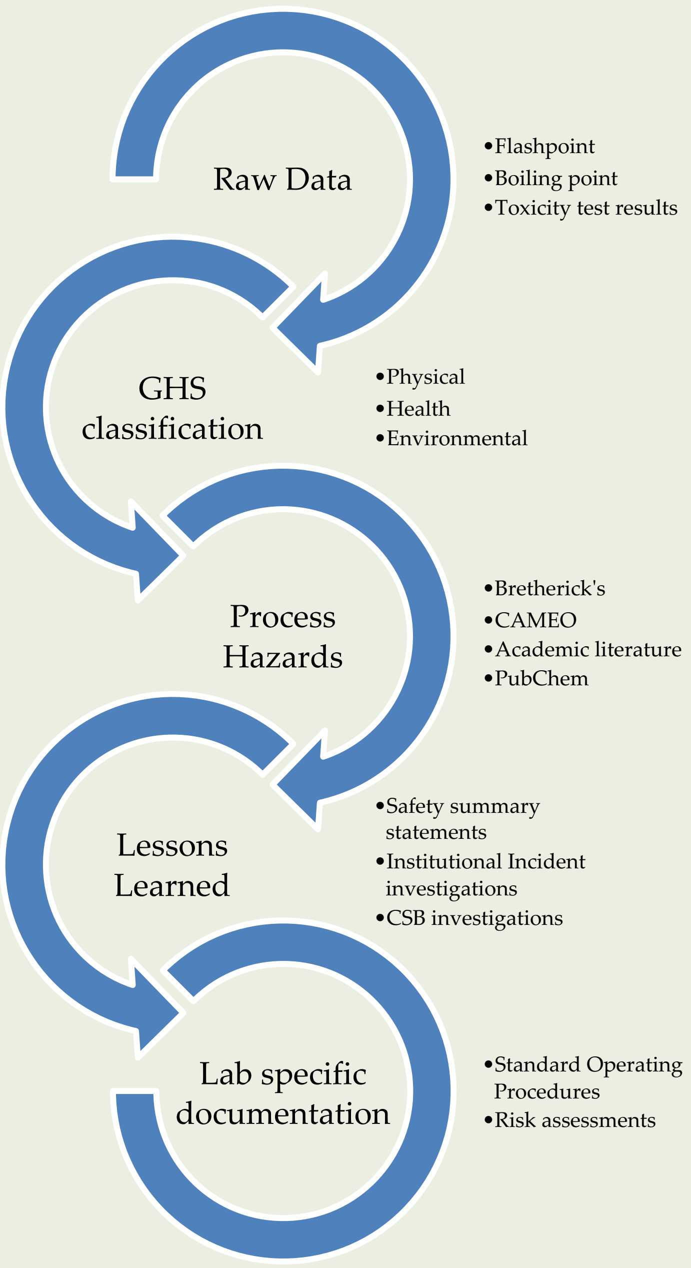
- …should inform readers about hazards requiring caution beyond common laboratory safety measures.
- …are intended to help those reproducing experiments to understand, mitigate, and prepare for unusual or special risks in reported methods.
- …will help organize and communicate safety information specific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

- "[D]iazo compounds can also explode… making them potentially dangerous to work with. Exactly how dangerous has been hearsay for a long time, since there haven't been any systematic studies on the hazards of these dinitrogen compounds."
  Chem. Engr. News. Dec 12, 2019, 97 (48).
- "None are predicted to be explosive, but many are predicted to exhibit impact sensitivity with exothermic decomposition… The principal hazard of using diazo compounds (ignoring toxicity), particularly sulfonyl azides… is the risk of thermal runaway and pressure generation."
  Org. Process Res. Dev. 2020, **24**, 1, 67–84.
  DOI: 10.1021/acs.oprd.9b00422
- "[C]omputational analysis demonstrated that hydrolysis of the sulfonyl azide bond was greatly favored thermodynamically. Although some sulfonyl azides are nonexplosive and nonhydroscopic, these kinetically stable compounds are similar to caged tigers which might be released by unpredictable factors over long-term storage."
  Org. Lett. 2013, **15**, 1, 18–21. DOI: 10.1021/ol3028708

Lessons Learning

- C&EN: diazos, to use or not to use…
- *misinformation thrives on lack of nuance*

- assess risk and communicate findings
  - need more documented analysis in research/experimental context
- cite sources (!)
  - provides provenance and others can follow up
- additional information literacy instruction
  - ACRL information literacy frames – all apply to safety information
    - Authority Is Constructed and Contextual
    - Information Creation as a Process
    - Information Has Value
    - Research as Inquiry
    - Scholarship as Conversation
    - Searching as Strategic Exploration



References & resources

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- ACS Center for Lab Safety (acs.org/safety)
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