Information Literacy in the Disinformation Era: Challenges in working with chemical safety information

Ralph Stuart, Keene State College
Leah McEwen, Cornell University
Sammye Sigmann, Appalachian State University
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?
Context is important in laboratory safety
RAMP: informed risk assessment

Recognize hazards – Using available information from chemical labels, SDSs, documented procedures, and 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

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

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


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

“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*

SDS excerpt (left) where the data was not carefully considered by the preparer.
Sodium azide

**Laboratory Chemical Safety Summary (LCSS) Datasheet**

Molecular Formula: $\text{NaN}_3$

Synonyms:
- sodium azide
- 26628-22-8
- Azide, sodium
- Natriumazid
- Sodiumazide

Molecular Weight: 65.01 g/mol
# Hydrazoic Acid (Compound LCSS)

## 1 GHS Classification

### Pictogram(s)

- Explosive
- Irritant
- Health Hazard

### Signal

**Danger**

- **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](#))

### GHS Hazard Statements


(The corresponding statement to each P-code can be found at the GHS Classification page.)

### Precautionary Statement Codes

- NITE-CMC

**Source:** NITE-CMC

**Record Name:** Hydrogen azide - E5200

**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).
### MyChemicals

#### MyChemicals Collection

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

#### Incompatibility Information

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Incompatible</th>
<th>Compatible</th>
</tr>
</thead>
<tbody>
<tr>
<td>SODIUM AZIDE</td>
<td>Explosive Generates gas Intense or explosive reaction Toxic</td>
<td></td>
</tr>
<tr>
<td>SULFURYL CHLORIDE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ACETONITRILE</td>
<td>Caution Flammable</td>
<td></td>
</tr>
<tr>
<td>ETHYL ACETATE</td>
<td>Caution</td>
<td></td>
</tr>
<tr>
<td>HYDROCHLORIC ACID, SOLUTION</td>
<td>Incompatible Explosive Generates gas Generates heat Intense or explosive reaction Toxic Unstable when heated</td>
<td></td>
</tr>
<tr>
<td>WATER</td>
<td>Incompatible Generates gas Generates heat</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Incompatible Corrosive Generates gas Generates heat Intense or explosive reaction Toxic</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Caution Flammable Generates gas Toxic</td>
<td></td>
</tr>
</tbody>
</table>

#### Reactivity Predictions

- View chemical datasheets (with respect to the name of any substance in the list)
- Consider the reactivity predictions if chemical's reactive hazards (including all chemical datasheet.)
- Generate a report (with reactivity predictions)

[Print Report]
Chemical Datasheet for **SULFURYL CHLORIDE**

### Hazards

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.

### 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


### Belongs to the Following Reactive Group(s)

- Acyl Halides, Sulfonyl Halides, and Chlorofomates

### 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

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
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…

- 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
Not all diazo compounds are hazardous...

...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 nonhygroscopic, 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
  o need more documented analysis in research/experimental context

• cite sources (!)
  o provides provenance and others can follow up

• additional information literacy instruction
  o 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

---

**Raw Data**
- Flashpoint
- Boiling point
- Toxicity test results

**GHS classification**
- Physical
- Health
- Environmental

**Process Hazards**
- Bretherick's
- CAMEO
- Academic literature
- PubChem

**Lessons Learned**
- Safety summary statements
- Institutional Incident investigations
- CSB investigations

**Lab specific documentation**
- Standard Operating Procedures
- Risk assessments
References & resources


• Sigmann, S. B.; McEwen, L. R. Teaching Chemical Safety and Information Skills Using Risk Assessment. In *Integrating Information Literacy into the Chemistry Curriculum*; Eds. Lovett, C. F.; Shuyler, K.; Li, Y. 2016, Ch 3. DOI: 10.1021/bk-2016-1232.ch003


• ACS Division of Chemical Health & Safety (dchas.org)
• ACS Center for Lab Safety (acs.org/safety)
  ➤ Workshops
  ➤ Courses
  ➤ Videos

Free online course
Foundations of Chemical Safety and Risk Management©
[learning.acs.org](http://learning.acs.org) (ACS Chemical Safety Program)