PubChem LCSS (Laboratory Chemical Safety Summary)

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Leah McEwen, Ralph Stuart
Lab Safety ...

.. an important and fundamental topic in chemistry labs
.. safety guidelines in every lab
.. chemical safety handbooks ..
.. accidents occurred from time to time
LCSS - Laboratory Chemical Safety Summary

• LCSS has been published to meet the lab safety needs

91 chemicals

88 chemicals

Needs for online resource for chemical safety information
In 2015, PubChem, together with health and safety professionals from CHAS, CINF, and universities, created an online version of LCSS. With several updates, the current PubChem LCSS is fully digitized and the data behind is fully machine readable.
Outline

• PubChem LCSS overview
• LCSS content
• LCSS updates
• LCSS data access and retrieval
• Summary
LCSS - Laboratory Chemical Safety Summary

• Subset of the PubChem compound summary

• Format of TOC - Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards (2011) + GHS + …
Data ... chemical centralized and beyond

- Chemical structure – 2D/3D, SMILES, InChI, SDF...
- Property - 
- Drug and medication
- Agrochemicals
- Food additives
- Safety and hazards
- Toxicity
- Literature
- Patents
- Bioactivity
- Target
- Natural products
- Pathways
- … more

LCSS
PubChem LCSS Contents

• Example: Acetone

1. Google/PubChem search … acetone
2. Launch the PubChem acetone page
3. Click the LCSS link
PubChem LCSS - acetone

PubChem LCSS Contents

• 12 main headings
• Each section may have multiple subheadings
• Each data item may have multiple values integrated from multiple sources.
PubChem LCSS Contents

Contents:
- Title and Summary
- 1 GHS Classification
- 2 Identifiers
- 3 Physical Properties
- 4 Toxicity Data
- 5 Exposure Limits
- 6 Health and Symptoms
- 7 First Aid
- 8 Flammability and Explosivity
- 9 Stability and Reactivity
- 10 Storage and Handling
- 11 Cleanup and Disposal
- 12 Information Sources

2 Identifiers

3 Physical Properties

- 3.1 Physical Description
- 3.2 Odor
- 3.3 Boiling Point
- 3.4 Melting Point
- 3.5 Flash Point
- 3.6 Solubility
- 3.7 Density
- 3.8 Vapor Density
- 3.9 Vapor Pressure
- 3.10 Autoignition Temperature
- 3.11 Odor Threshold

4 Toxicity Data

5 Exposure Limits

6 Health and Symptoms
PubChem LCSS – Total LCSSs

- More than 120,000 LCSS pages
- 2015 – 3,000
- 2017 – 5,000
- 2018 – 108,000
- 2019 – 122,000
Jyllian: There’s all sorts of possible tools. Not everything has all the information. I think possibly the closest you might come to that is PubChem, which has safety information. In particular with PubChem, one of the things I really appreciate is that it tracks back where it got that information from, so you can see the source and evaluate how applicable what that particular source did is to your situation.
LCSS Data and Provenance

• LCSS data are integrated from many sources
• The data source link allows users to track back the original data site.

E.g. GHS for toluene:

LCSS Data and Provenance
PubChem GHS Summary

GHS Classification

GHS, the Globally Harmonized System of Classification and Labeling of Chemicals, was developed by the United Nations as a way to bring into agreement the chemical regulations and standards of different countries. GHS includes criteria for the classification of health, physical and environmental hazards, as well as specifying what information should be included on labels of hazardous chemicals as well as safety data sheets. This page summarizes the relationship of GHS hazard statements, pictograms, signal words, hazard classes, categories, and precautionary statements.

Ref: UNECE GHS (Rev.7) (2017)

Hazard Class Pictograms

- **Explosive**: 
  - Exploding Bomb
  - Explosives
  - GHS01
- **Flammable**: 
  - Flame
  - Flammable
  - GHS02
- **Flame Over Circle**: 
  - Oxidizer
  - GHS03
- **Gas Cylinder**: 
  - Gas Cylinder
  - Compressed Gases
  - GHS04
- **Corrosive**: 
  - Corrosion
  - Corrosives
  - GHS05
- **Exclamation Mark**: 
  - Irritant
  - GHS07
- **Health Hazard**: 
  - Health Hazard
  - GHS08
- **Skull and Crossbones**: 
  - Skull and Crossbones
  - Acute Toxicity
  - GHS06
- **Environment**: 
  - Environment
  - GHS09

Note: All pictograms are shown in svg format in the page. The corresponding gif images are also available, e.g. https://pubchem.ncbi.nlm.nih.gov/images/ghs/GHS08.gif
LCSS Updates

- Webpage layout (look and feel).
- Backend data: the backend data format has a significant change.
- Reduced the page size for default display:
  - A LCSS page showing only 1 or 2 values for most data headings, users can view additional values by clicking the expand icon.
- Added reactivity alerts.
- Added NFPA 704 diamond.
- Added GHS “not classified” category
Acetone

PubChem CID: 180

Chemical Names: Acetone; 2-propanone; Propanone; 67-64-1; Dimethyl ketone; Methyl ketone
Molecular Formula: C3H6O; CH3-CO-CH3
Molecular Weight: 58.08 g/mol

1 GHS Classification

Signal: Danger
GHS Hazard Statements
H225: Highly flammable liquid and vapor (Danger)
H319: Causes serious eye irritation (Warning)
H336: May cause drowsiness or dizziness (Warning)

Precautionary Statement Codes
P210, P233, P240, P241, P242, P243, P261, P264, P337+P313, P370+P378, P403+P233, P403+P22, (The corresponding statement to each P-code c

Structure:

Chemical Names:
- acetone
- 2-propanone
- propanone
- 67-64-1
- Dimethyl ketone
- Methyl ketone

Molecular Formula: C3H6O or CH3-CO-CH3 or CH3COCH3
Molecular Weight: 58.08 g/mol
LCSS Updates – Backend data

• No more HTML markup within strings, instead, we have an explicit markup object that separates primary strings from the various markup types. No more embedded tables in the data blobs.

• All HTML entities are replaced by UTF-8 characters, e.g. \&alpha; \&945; or \&x3B1; → α.

LCSS Updates – Backend data spec

• Data blob specification:

LCSS Updates – Page size reduced

Reduced the data volume for default display:
- A LCSS page showing only 1 or 2 values for each data item, users can view additional values by clicking the expand icon.

CID 180

Acetone

Boiling Point

133 °F at 760 mm Hg (NTP, 1992)
- from CAMEO Chemicals

55.75°C
- from EPA DSSTox

56.08 deg C
- from HSDB

56 °C
- from ILO-ICSC

133°F
- from OSHA Occupational Chemical DB: The National Institute for Occupational Safety and Health (NIOSH)
# LCSS Updates – reactivity alerts

## 9.3 Reactivity Alerts

### Highly Flammable
- from CAMEO Chemicals

### 9.3.1 CSL Reaction Information

<table>
<thead>
<tr>
<th>CSL No</th>
<th>CSL00003</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactants/Reagents</td>
<td>ACETONE; sodium percarbonate</td>
</tr>
<tr>
<td>Reaction Class</td>
<td>Oxidation</td>
</tr>
<tr>
<td>GHS Category</td>
<td>Explosive</td>
</tr>
<tr>
<td>Reaction Scale</td>
<td>5 (up to 1g)</td>
</tr>
<tr>
<td>Warning Message</td>
<td>Can form explosive acetone peroxide compounds</td>
</tr>
<tr>
<td>Source Reference</td>
<td>User-Reported</td>
</tr>
<tr>
<td>CSL Status</td>
<td>Approved</td>
</tr>
<tr>
<td>Additional Info</td>
<td>Bassan et al OPRD 2013, 17, 1611-1616</td>
</tr>
<tr>
<td>Modified Date</td>
<td>2/27/2016</td>
</tr>
</tbody>
</table>

- from Pistoia Alliance Chemical Safety Library

### 9稳定性 and Reactivity
- 9.1 Hazardous Reactivities & Incompatibilities
- 9.2 Reactivity Profile
- 9.3 Reactivity Alerts
  - 9.3.1 CSL Reaction Information

### CONTENTS
- Title and Summary
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- 9 Stability and Reactivity
  - 9.1 Hazardous Reactivities & Incompatibilities
  - 9.2 Reactivity Profile
  - 9.3 Reactivity Alerts
### 8.4 NFPA Hazard Classification

<table>
<thead>
<tr>
<th>NFPA 704 Diamond</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 3 0 1-3-0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>NFPA Health Rating</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Materials that, under emergency conditions, can cause significant irritation.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>NFPA Fire Rating</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Liquids and solids that can be ignited under almost all ambient temperature conditions. Materials produce hazardous atmospheres with air under almost all ambient temperatures or, though unaffected by ambient temperatures, are readily ignited under almost all conditions.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>NFPA Instability Rating</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Materials that in themselves are normally stable, even under fire conditions.</td>
</tr>
</tbody>
</table>

From HSDB
### Summary of Classification and Labelling

#### Notified classification and labelling

<table>
<thead>
<tr>
<th>EC / List no.</th>
<th>Name</th>
<th>CAS Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>231-791-2</td>
<td>Water</td>
<td>7732-18-5</td>
</tr>
</tbody>
</table>

#### Notified classification and labelling according to CLP criteria

<table>
<thead>
<tr>
<th>Classification</th>
<th>Hazard Class and Category Code(s)</th>
<th>Hazard Statement Code(s)</th>
<th>Supplemental Hazard Statement Code(s)</th>
<th>Pictograms, Signal Word Code(s)</th>
<th>Specific Concentration Limits, M-P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Not Classified</td>
<td></td>
<td></td>
<td></td>
<td>GHS05 GHS07 Dgr</td>
<td></td>
</tr>
<tr>
<td></td>
<td>H302</td>
<td>H318</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flam. Liq. 3</td>
<td>NA</td>
<td>H226</td>
<td>H226</td>
<td>GHS02 Wng</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Not Classified</td>
<td></td>
<td></td>
<td></td>
<td>GHS05 Dgr</td>
<td></td>
</tr>
<tr>
<td>Acute Tox. 3</td>
<td>H301</td>
<td>H301</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Corrosion**: Not classified
- **Flame**: Not classified
- **Skull and crossbones**: Not classified
- **State/Form IUPAC Names**: Not classified
- **Joint Entries**: 1157
- **Number of Notifiers**: 2
- **State/Form**: 1
LCSS Updates – GHS “not classified”
LCSS Data access and retrieving

• Web pages – URL or scan QR code
• Pug_view to get data blob
• For data under specific heading, using pug_view + heading
• FTP
LCSS Data access and retrieving

• Web pages – URL or scan QR code
  ✔ URL: search engine, or direct URL
  ✔ QR code generator:

LCSS Data access and retrieving

• Programmatic users: Pug_view to get data blob

✓ Get all page data for a given compound:

✓ Get partial page data for specific headings:
LCSS Data – programmatic access
LCSS Data access and retrieving

Summary

• PubChem created the LCSS aiming to help lab researchers, hygiene officers, and students to locate the chemical safety and hazard information.

• PubChem LCSS data are integrated from many authoritative sources, and all data can be tracked back to the original source.

• LCSS information can be accessed and retrieved in multiple methods.
Thank you ...

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