

# Using a chemical inventory system to optimize safe laboratory research

GRACE BAYSINGER, R. KEVIN CREED, AND LARRY GIBBS

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CHEMICAL, SAMPLE & ASSET MANAGEMENT TOOLS

DIVISION OF CHEMICAL HEALTH AND SAFETY

ACS NATIONAL MEETING IN SAN DIEGO

WEDNESDAY, MARCH, 16, 2016 FROM 11:15 AM - 11:40 AM



# Goal: Getting from here to there



## Non-Waste Hazardous Materials Inventory Statement

For use by Unidocs Member Agencies or where approved by your Local Jurisdiction



<b>Business Name:</b> Leland Stanford Junior University				<b>Type of Report on This Page:</b> <input type="checkbox"/> Add; <input type="checkbox"/> Delete; <input type="checkbox"/>				
<b>Chemical Location:</b> CHEMISTRY NON_COMPLY (Demo)			<b>EPCRA Confidential Location?</b> <input type="checkbox"/> Yes; <input type="checkbox"/> No		<b>Facility ID#(Agency Use Only)</b>			
			<b>Trade Secret Information?</b> <input type="checkbox"/> Yes; <input type="checkbox"/> No					
Haz. Class	Map and Grid or Location Code	Common Name	Hazardous Components (For mixtures only)		Type and Physical State	Quantities		
			Wt.	Chemical Name EHS CAS No.		Max. Daily	Average Daily	Largest Container
2.2	177, 355, 189, 327, 366, 325	Argon, gas CAS No.: 7440-37-1 <input type="checkbox"/> EHS			pure gas	4074 <b>Curies:</b>	4074 <b>Days On Site:</b> 365	336 <b>Storage Container:*</b> L
2.2	352	Carbon dioxide, compressed gas CAS No.: 124-38-9 <input type="checkbox"/> EHS			pure gas	570 <b>Curies:</b>	570 <b>Days On Site:</b> 365	570 <b>Storage Container:*</b> L
2.3	177	Chlorine dioxide, gas CAS No.: 10049-04-4 <input type="checkbox"/> EHS			pure gas	600 <b>Curies:</b>	600 <b>Days On Site:</b> 365	300 <b>Storage Container:*</b> L

# Occupational Health + Safety Services



*and to here*

Stanford University Compatible Storage Group Classification System  
Should be used in conjunction with specific storage conditions taken from the manufacturer's label and MSDS.

### STORAGE GROUPS

Store chemicals in separate secondary containment and cabinets  
Find Storage Group information in Chemtracker:  
<https://chemtracker.stanford.edu/chemsafety>

- A** Compatible Organic Bases
- B** Compatible Pyrophoric & Water Reactive Materials
- C** Compatible Inorganic Bases
- D** Compatible Organic Acids
- E** Compatible Oxidizers including Peroxides
- F** Compatible Inorganic Acids not including Oxidizers or Combustible
- G** Not Inherently Reactive or Flammable or Combustible
- J\*** Poison Compressed Gases
- K\*** Compatible Explosive or other highly Unstable Material
- L** Non-Reactive Flammable and Combustible, including solvents
- X\*** Incompatible with ALL other storage groups

**\*Storage Groups J, K and X: Contact EH&S @ 3-0448  
For specific storage - consult manufacturer's MSDS**

If space does not allow Storage Groups to be kept in separate cabinets the following scheme can be used with extra care taken to provide stable, uncrowded, and carefully monitored conditions.

Storage Group X must be segregated from all other chemicals.

Storage Group B is not compatible with any other storage group.



# Major Issues Driving Business Needs

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## Safety

- Lab accident with injuries
- Property damage
- Lab fire
- Delayed spill response

## Resource Management

- Excess purchasing
- No waste minimization
- Excess space allocation
- Fire code occupancy type

## Compliance

- OSHA citations
- Hazard communication
- Lab standard – Standard operation procedures
- Hazardous materials information system
- Community right to know violations



# Business Needs Affect System & Resource Requirements

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## System Configuration

- Paper / index cards
- Spreadsheets
- Access or other in-house databases
- Commercial off-the-shelf, local installation
- Software as a service (SaaS), client hosted
- Software as a service (SaaS), vendor hosted

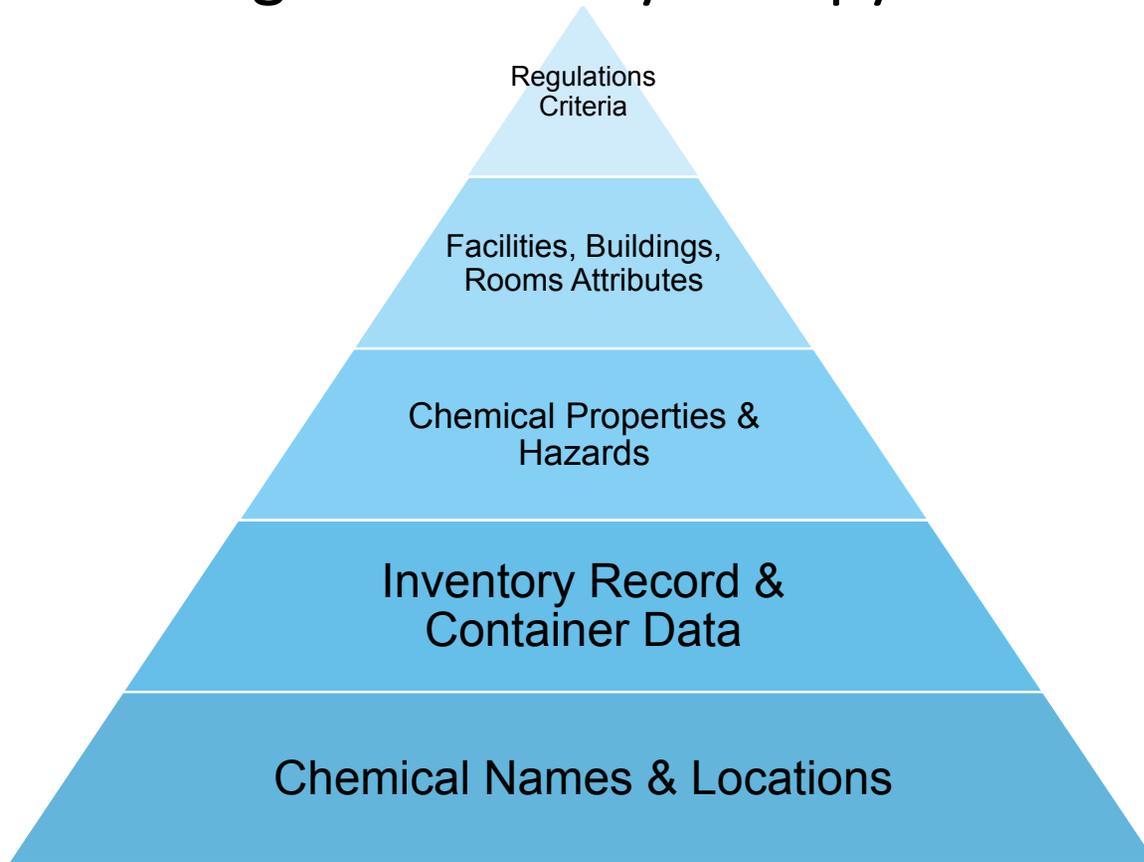
## Support Resources

- Client IT vs Vendor IT
- Highly centralized vs decentralized
- Administrative support
- Small-to-medium enterprise support

## User Groups

- Lab Researchers, Principal investigators, Managers
- Facilities personnel
- EH&S professionals
- Fire code compliance
- Emergency response personnel

# Building an inventory data pyramid



**HMIS, SARA, EPCRA Reports  
CFATS Screening  
Fire / Building Code / NFPA  
Compliance**

**Control Area Designations  
Project Planning – Occupancy Type  
Determination  
Sprinkler & Cabinet Credits  
Lab Safety Inspections**

**Expanded Search Capabilities  
Lab STD – SOPs, PHS Evaluations  
Safe Segregation in Storage  
Oversight of Extremely Hazardous  
Chemicals**

**Record Management  
Tracking Critical Expiration Dates  
Unique Identifiers – Barcode  
Numbers**

**Basic Inventory  
Partial Hazard communication**

# Extensive Inventory Record Fields Add Value

---

## **User Entered - Basics**

- Department
- Building
- Room
- Owner
- Chemical Name
- Physical State
- Amount
- Units
- Number of Same-size Containers

## **System Generated**

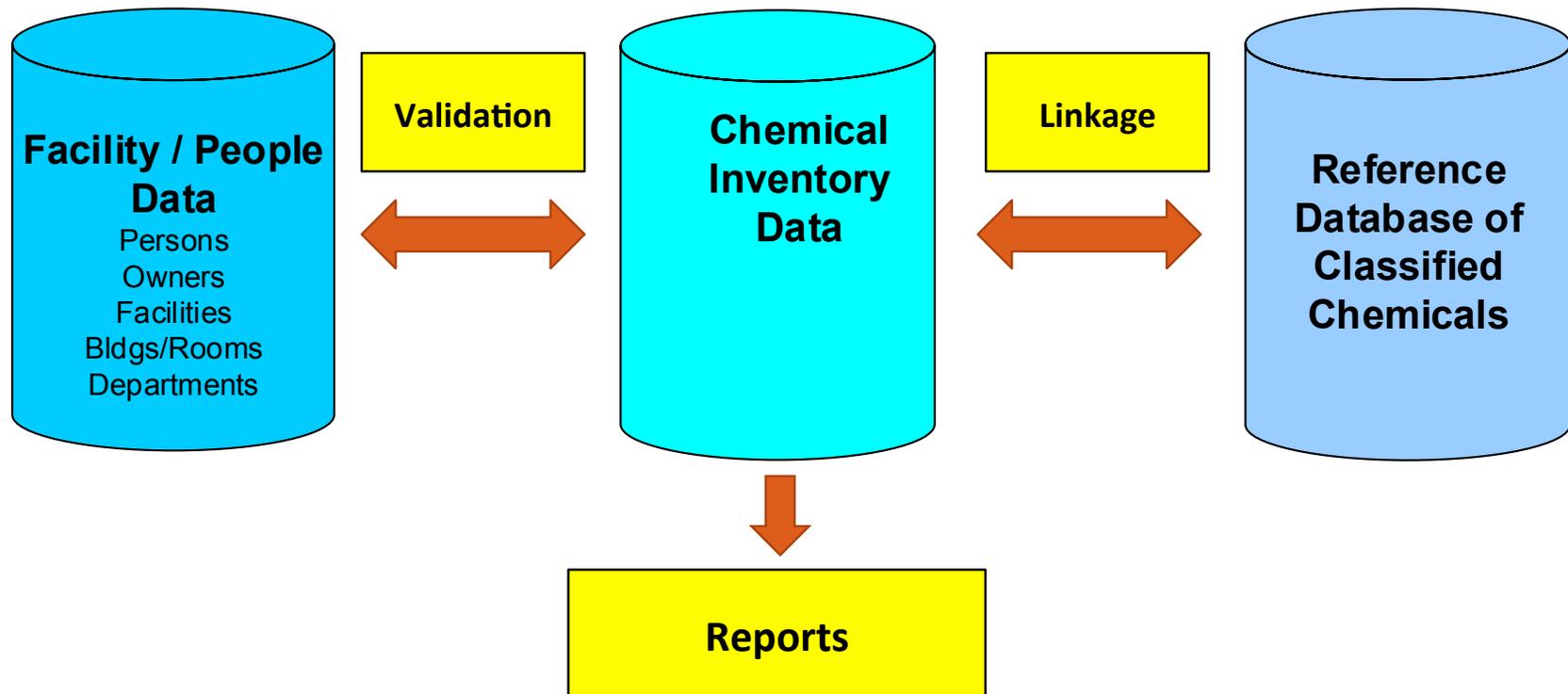
- Created by/date
- Modify by/date
- Storage group
- Record number

## **Other Inventory Fields**

- Floor
- Bay/bench
- Shelf
- Location
- Barcode number
- User defined fields
- Surplus
- CAS number

- Formula
- Manufacturer
- Product number
- Received date
- Inventoried by
- Expiration date

# Linkage to Reference Data and Validation of Inventory Data Creates Bridge to Reports



# Effective Bridging Inventory Data to Reports Depends Upon **Accuracy** of Data

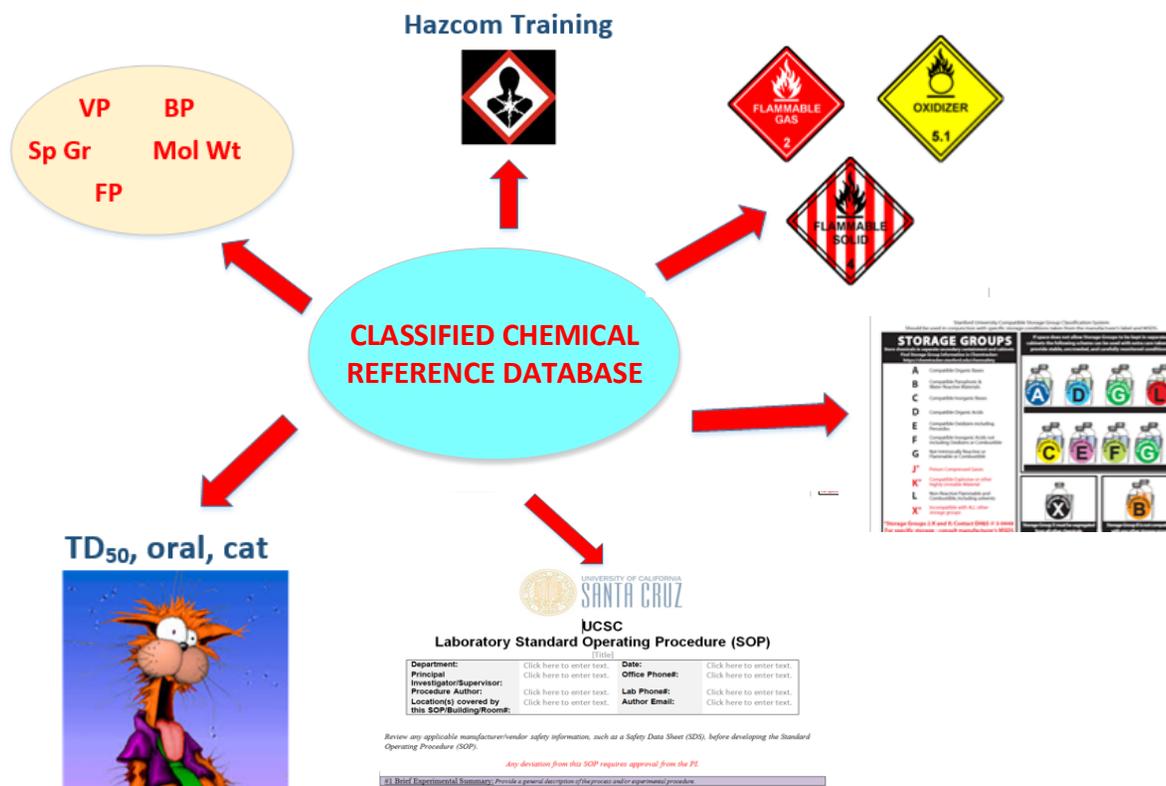
---



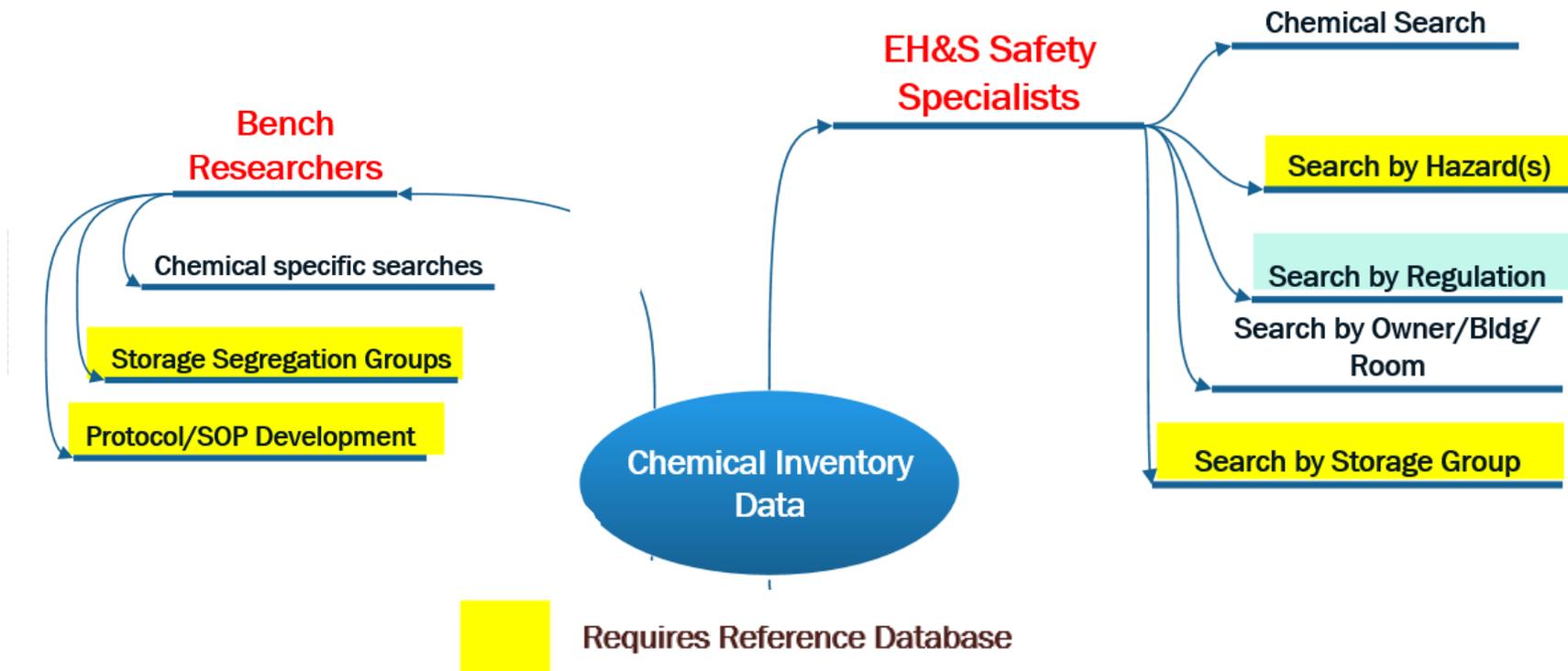
- **Centralized vs Decentralized**
- **Linkage to Reference Data**

(Ref: JCHS, May/June 2012; D. Quigley, et.al.)

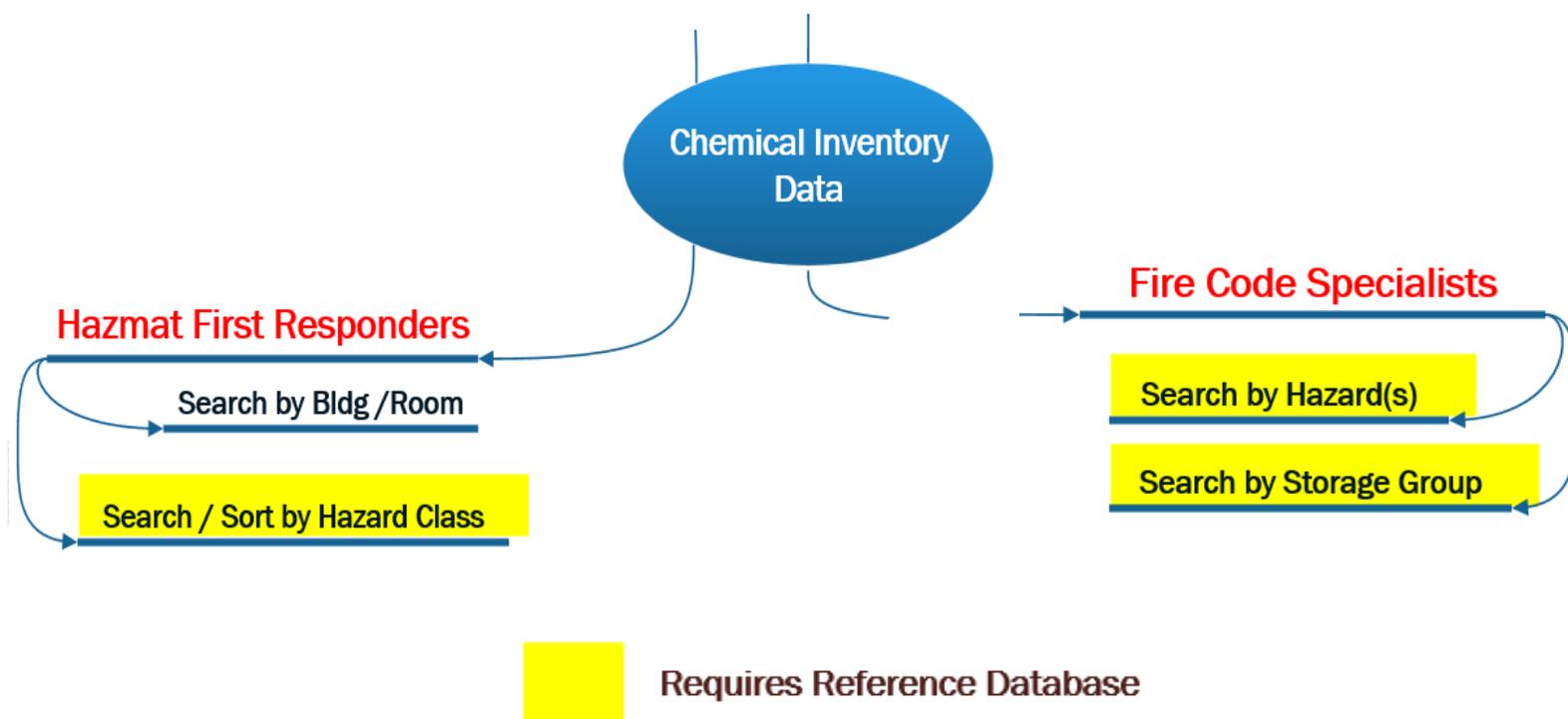
# Classified Chemical Reference Database Supports Hazard Identification, Safe Segregation, Lab Standard Compliance



# Logistical Considerations – Users



# Logistical Considerations – Users



# ChemTracker

ChemTracker



## Welcome to ChemTracker 4 Inventory Management

Enter username and password to continue.

[Forgot password](#)

*If you are having difficulties logging in, please contact your local  
ChemTracker Administrator.*

© ChemTracker® is a registered Service Mark of the Board of Trustees of Leland Stanford Junior University

# Inventory Search – Chemical / Material ID

ChemTracker Home **Search** Add ChemInfo graceb Help

Search

Inventory Search [Access Search Templates](#)

▼ **Chemical / Material ID**

Chemical Identifier: *Choose One*  *Chemical Name*  *Formula*  *CAS Number*  *GDN*  
 *Begins with*  *Contains*  *Equals* [?](#)

Manufacturer  Product Number

Physical State

# Inventory Search – Location

ChemTracker Home **Search** Add ChemInfo graceb Help

**Search**

Inventory Search [Access Search Templates](#)

▼ **Location**

<b>Building</b>	<input type="text"/>	<b>Department</b>	<input type="text"/>
<b>Room</b>	<input type="text" value="Select a building to enable"/>	<b>Floor</b>	<input type="text" value="Select a building to enable"/>
<b>Bay / Bench</b>	<input type="text" value="Select a building and room to enable"/>	<b>Control Area</b>	<input type="text" value="Select a building to enable"/>
<b>Location</b>	<input type="text"/>	<b>Shelf</b>	<input type="text"/>

# Inventory Search – Owner / Container Information

**ChemTracker**   Home   **Search**   Add   ChemInfo   graceb   Help

**Search**

Inventory Search   [Access Search Templates](#)

▼ **Owner / Container Information**

Owner	Container Barcode/s   (0 / 1000 barcodes)	<input type="button" value="Browse..."/>
<input type="text"/>	<input type="text" value="Total of 1000 barcodes allowed"/>	
Inventoried By		
<input type="text"/>		
Inventory ID		
<input type="text"/>		

# Inventory Search – Regulation / Hazard / Storage

ChemTracker Home **Search** Add ChemInfo graceb Help

**Search**

Inventory Search [Access Search Templates](#)

▼ **Regulation / Hazard / Storage**

Storage Group	Hazard Group ?
<input type="text"/>	<input type="text"/>
Regulation Type	Regulation Class
<input type="text"/>	Select a regulation type first
Regulation ID	
Select a regulation type and class first	

# Inventory Search – Record Data & User Defined Fields

ChemTracker Home **Search** Add ChemInfo graceb Help

**Search**

Inventory Search [Access Search Templates](#)

▼ **Record Data**

Expiration Date	Modified Date
Before ▾ mm/dd/yyyy 	Before ▾ mm/dd/yyyy 
Received Date	Modified By
Before ▾ mm/dd/yyyy 	<input type="text"/>

▼ **User Defined Fields**

UDF1	UDF2
<input type="text"/>	<input type="text"/>
UDF3	
<input type="text"/>	

[Show / hide all categories](#) [Save search](#) [Search](#) [Clear selections](#)

# ChemInfo Reference Database

## ChemInfo

Chemical Identifier: Choose One  Chemical Name  Formula  CAS Number  GDN

Begins with  Contains  Equals ?

PHOSGENE (20% IN TOLUENE)

phosgene

- phosgene
- PHOSGENE
- PHOSGENE (20% IN TOLUENE)
- PHOSGENE (COMPRESSED GAS)
- PHOSGENE <0.10% IN INERT CARRIER GAS
- PHOSGENE DIPHENYL ACETAL
- PHOSGENE IMINIUM CHLORIDE
- PHOSGENE SOLUTION (20% IN TOLUENE)

# ChemInfo Search Results

ChemTracker Home Search Add **ChemInfo** graceb Help

## ChemInfo

Chemical Identifier: Choose One  Chemical Name  Formula  CAS Number  GDN  
 Begins with  Contains  Equals ?

PHOSGENE (20% IN TOLUENE)

You searched for: Chemical Name Begins with PHOSGENE (20% IN TOLUENE)

Showing all 1 rows. ?

Actions	Chemical Name	Physical State
<a href="#">ChemInfo</a> <a href="#">SDS</a>	PHOSGENE (20% IN TOLUENE)	L

# ChemInfo Record for Phosgene Solution (20% in Toluene)

## ChemTracker

### ChemInfo Details

#### Chemical

PHOSGENE SOLUTION (20% IN TOLUENE)

Storage Group: L: Flammables and Combustibles, including solvents

#### Storage Conditions

SARA 312 Pressure: Ambient

SARA 312 Temperature: < Ambient but not cryogenic

#### NFPA Classifications

REACTIVITY 0

FIRE 3

HEALTH 3

#### Physical Properties

DENS: .935 g/cm<sup>3</sup>

FP: 4 C

#### Fire Codes

UFC VI-A-Health: Corrosives, Acids

UFC VI-A-Health: Highly toxic materials (solid or liquid)

UFC VI-A-Physical: Flammable Liquids Class IB Flash point <73° F and BP >100° F

#### Hazards

3 - Flammable liquid (main hazard)

12 - Severely toxic

15 - Flammable

21 - Corrosive

33 - Lachrymator

37 - Hepatotoxin

38 - Nephrotoxin

43 - Mucous membrane damage

66 - California Prop. 65 Reproductive toxin

72 - Teratogen

# ChemInfo Record for Phosgene Solution (20% in Toluene) continued

## Regulations

DOT-Hazard Class 2nd: DOT Flammable Liquids

DOT-Hazard Class or Div.: DOT Toxic substances.

DOT-PACKING GROUP: DOT Packing Group 1

IBC-Health: IBC Highly Toxic (LD50 < 50 oral or < 200 Derm) MG/KG or LC50 < 200 PPM inhail

IBC-Physical: IBC Flammable Liquid IB FP <73° F and BP >100° F

IBC-Physical: IBC Flammable Liquid class IA, IB and IC Combination

Local-NYC-SARA-RTK: NYC Right-to-Know, definition based

NGO-IARC: IARC Carcinogen Group 3: not classifiable as to its carcinogenicity to humans.

SARA-HAZ: Delayed health effects: US EPA SARA 312

SARA-HAZ: Flammable: US EPA SARA 312312

SARA-HAZ: Immediate health effects: US EPA SARA 312

US-EPA: RCRA 261.21 Characteristic of ignitability

## Toxicology

### Synonyms

DOT Toxic by inhalation liquid, flammable, n.o.s.

MAIN Phosgene solution (20% in toluene)

SYNONYM Phosgene (20% in Toluene)

### Additional Identifiers

MDL NUM MFCD00036119

UN/NA UN3384



# Searching Multiple Lab Safety Resources at one time – a Prototype



STANFORD  
UNIVERSITY  
LIBRARIES

Full Record

Title

Author

Date Range

From  To

Match

Limit to Available Full-Text

Clear

Search

- All Categories
- Databases
- eBooks & eJournals
- MSDS
- Regulatory
- Safety Data
- Syntheses & Reactions
- Websites

All Categories

**Databases**

- Engineering Village
- Environmental Sciences & Pollution Management
- Health & Safety Sciences Abstracts
- PubMed
- Scopus
- Web of Science Core Collection

**eBooks & eJournals**

- ACS Publications
- ACS Symposium Series
- CRCnetBASE
- eBrary
- MyiLibrary
- National Academies Press
- ProQuest Dissertations & Theses Global
- ProQuest Research Library
- RSC Journals
- ScienceDirect
- SpringerLink
- Wiley eBooks
- Wiley Online Library

**MSDS**

- MSDS (CCOHS)
- MSDSonline

**Regulatory**

- Cal/OSHA
- U.S. Chemical Safety Board
- U.S. Environmental Protection Agency
- U.S. Occupational Safety and Health Administration

**Safety Data**

- ACToR (Aggregated Computational Toxicology Resource)
- CAMEO Chemicals
- Canadian Centre for Occupational Health and Safety (Web Information Service)
- Chemical Safety Database
- ChemID Plus Advanced
- e-EROS : Encyclopedia of Reagents for Organic Synthesis - Chemical Name
- Emergency Response Safety and Health Database
- Hazardous Substances Data Bank
- INCHEM
- International Chemical Safety Cards (ICSC) database
- Knovel
- NIOSH Pocket Guide to Chemical Hazards
- PubChem - Compound Search
- WebWISER-Known Substance List

**Syntheses & Reactions**

- CAMEO Chemicals
- e-EROS : Encyclopedia of Reagents for Organic Synthesis - Chemical Name
- Organic Reactions
- Organic Syntheses
- Science of Synthesis

**Websites**

- ACS Division of Chemical Health and Safety
- Berkeley EH&S
- Caltech EH&S
- Columbia University EH&S
- Cornell EH&S
- Harvard EH&S
- MIT EH&S
- Princeton Univ EH&S
- Stanford EH&S
- UC Center for Laboratory Safety
- Yale EH&S

# Search Results for Phosgene

phosgene Options Search New Search About Sign In

Search: Full Record: phosgene (0) [Icons]

STANFORD UNIVERSITY LIBRARIES

Search Summary  
2,141 top results from 44,071 found in all sources  
49 of 49 sources complete

Topics Visual

All Results (2,151)

- ▼ Topics
  - ▶ Reaction (233)
  - ▶ Chemical (211)
  - ▶ Exposure (133)
  - ▶ Chemistry (57)
  - ▶ Organic Compounds (54)
- ▼ Authors
  - Senet, J.-P. G. (21)
  - Nagle, A. S. (14)
  - Sciuto, AM (14)
  - Jung, K. W. (14)

All (2,151) Databases (429) eBooks (555) eJournals (422) MSDS (62) Regulatory (60) Safety Data (409) Reactions (235) Websites (59)

Results 1 - 20 of 2,151 Sort by: Rank Limit to: All Collections

**Phosgene**

G. Malcolm. Dyson  
1927-01-01  
Chem. Rev.  
DOI: 10.1021/cr60013a003  
ACS Publications

**Phosgene**

Kirby E. Jackson  
1933-01-01  
J. Chem. Educ.  
DOI: 10.1021/ed010p622  
ACS Publications

**Phosgene**

1999-01-01  
Handbook of Compressed Gases  
DOI: 10.1007/978-1-4615-5285-7  
SpringerLink

**Phosgene**

1990-01-01  
Handbook of Compressed Gases

**Phosgene**<sup>[1]</sup>

**Names**

JUPAC name  
Carbonyl dichloride

Other names  
CG; carbon dichloride oxide; carbon oxychloride; Chloroformyl chloride; dichloroformaldehyde; dichloromethanone; dichloromethanal

**Identifiers**

CAS Number	75-44-5
ChEBI	CHEBI:29365
ChemSpider	6131
EC Number	200-870-3
Jmol interactive 3D	image
PubChem	6371
RTECS number	SY5600000
UNII	117K140075
UN number	1076
InChI	
InChI=1S/CCl2O/c2-1(3)4	
Key: YGYAW/DWMA/BLBF-UHFFFAOYSA-N	
InChI=1/CCl2O/c2-1(3)4	

# Search Results – Visual Wheel

Search: Full Record: phosgene Create new alert from this search



STANFORD  
UNIVERSITY  
LIBRARIES

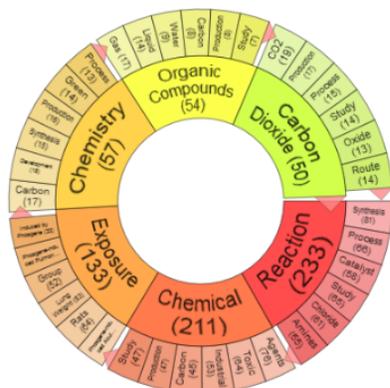
## Search Summary

2,141 top results from 44,071 found in all sources

49 of 49 sources complete

Topics Visual

All Results



All (2,151)	Databases (429)	eBooks (555)	eJournals (422)	MSDS (62)	Regulatory (60)	Safety Data (409)	Reactions (235)	Websites (59)
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SpringerLink

### Phosgene

1990-01-01  
Handbook of Compressed Gases  
DOI: 10.1007/978-1-4613-0673-3  
SpringerLink

### phosgene

Daintith, John; Martin, Elizabeth  
2010-01-01

## Phosgene<sup>[1]</sup>



### Names

**IUPAC name**  
Carbonyl dichloride

**Other names**  
CG; carbon dichloride oxide; carbon oxychloride; Chloroformyl chloride; dichloroformaldehyde; dichloromethanone; dichloromethanal

### Identifiers

**CAS Number** 75-44-5 ✓  
**CHEBI** CHEBI:29365 ✓  
**ChemSpider** 6131 ✓  
**EC Number** 200-870-3  
**Jmol interactive 3D** Image ✓  
**PubChem** 6371 ✓  
**RTECS number** SY560000  
**UNII** 117K140075 ✓  
**UN number** 1076

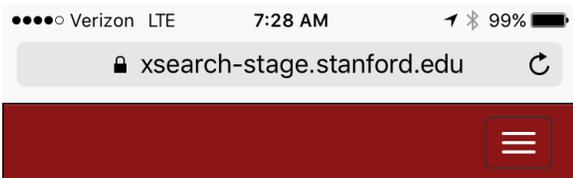
**InChI**  
InChI=1S:CCl2O/c2-1(3)4 ✓  
Key: YGYAWDWMABLBF-UHFFFAOYSA-N ✓  
InChI=1/CCl2O/c2-1(3)4  
Key: YGYAWDWMABLBF-UHFFFAOYAH

### SMILES

ClC(Cl)=O

### Properties

**Chemical formula** COCl<sub>2</sub>  
**Molar mass** 98.92 g mol<sup>-1</sup>



STANFORD  
UNIVERSITY  
LIBRARIES

Full Record

Title

Author

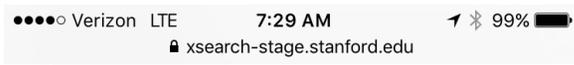
Date Range

From  To

Match

All

Limit to Available Full-Text



Title

Author

Date Range

From  To

Match

All

Limit to Available Full-Text

Clear

Search

All Categories

Databases

eBooks & eJournals

MSDS

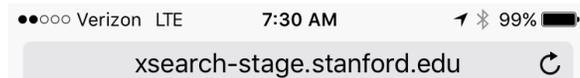
Regulatory

Safety Data

Syntheses & Reactions

Websites

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Phosgene

Search



All (2251)

Databases (431)

eBooks (606)

eJournals (422)

MSDS (62)

Regulatory (107)

Safety Data (409)

Reactions (235)

Websites (59)

CAS RN: 75-44-5

MSDSonline

Manufacturer: Air Liquide Canada Inc.

Show More

Phosgene PDF

MSDSonline

Manufacturer: Sigma-Aldrich Corporation

Show More

Phosgene PDF

MSDSonline



Go Back

### Filter Results: Safety Data

#### Filter by Collection

Limit to: All Collections

#### Filter by Topic

All Results (409)

##### ▼ Topics

- ▶ Organic Compounds (56)
- ▶ Carbonic Dichloride (43)
- ▶ Gas (17)
- Chloroformate (15)

Emergency Response Safety and He...  
INCHEM  
Knovel  
NIOSH Pocket Guide to Chemical...  
PubChem - Compound Search

Phosgene Search



### Safety Data

<<< < 1 > >>>

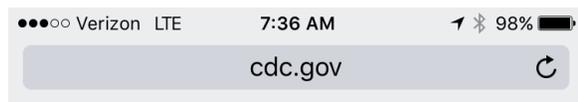
Results 1 - 15 of 15

[Index of ...](#)  
Index of Chemical Names, Synonyms and Trade Names. ... **Phosgene**\* 75-44-5 : SY5600000 : Phosphaniline: [Read More...](#)  
NIOSH Pocket Guide to Chemical Hazards

[Endrin](#)  
Endrin Synonyms & Trade ... parathion [Note: M emit hydrogen chloride & **phosgene** when heated or [Read More...](#)  
NIOSH Pocket Guide to Chemical Hazards

[Carbon tetrachloride - CDC](#)  
Carbon tetrachloride Synonyms & Trade Names

<a href="#">Phenyl mercaptan</a>	10
<a href="#">Phenyl methane</a>	10
<a href="#">N-Phenylmethylanine</a>	10
<a href="#">Phenyl-β-naphthylamine</a>	13
<a href="#">N-Phenyl-β-naphthylamine*</a>	13
<a href="#">4-Phenylnitrobenzene</a>	92
<a href="#">p-Phenylnitrobenzene</a>	92
<a href="#">Phenyl oxide</a>	10
<a href="#">Phenyl phosphate</a>	11
<a href="#">Phenylphosphine*</a>	63
<a href="#">2-Phenyl propane</a>	98
<a href="#">2-Phenyl propylene</a>	98
<a href="#">Phlogopite</a>	12
<a href="#">Phorate*</a>	29
<a href="#">Phosdrin*</a>	77
<a href="#">Phosgene*</a>	75
<a href="#">Phosphaniline</a>	63
<a href="#">Phosphine*</a>	78
<a href="#">Phosphorated hydrogen</a>	78
<a href="#">Phosphoric acid*</a>	76
<a href="#">Phosphoric acid (aqueous)</a>	76
<a href="#">Phosphoric chloride</a>	10
<a href="#">Phosphorus chloride [Phosphorus oxychloride]</a>	10
<a href="#">Phosphorus chloride [Phosphorus trichloride]</a>	77



Centers for Disease Control and Prevention  
Saving Lives. Protecting People.™

### Guide to Chemical Hazards

Search the NIOSH Pocket Guide

SEARCH

Enter search terms separated by spaces.

Phosgene

**Synonyms & Trade Names** Carbon oxychloride, Carbonyl chloride, Carbonyl dichloride, Chloroformyl chloride

CAS No. 75-44-5	RTECS No. SY5600000	DOT ID & Guide 1076 125
Formula COCl <sub>2</sub>	Conversion 1 ppm = 4.05 mg/m <sup>3</sup>	IDLH 2 ppm See: 75445

**Exposure Limits** NIOSH REL : TWA 0.1 ppm (0.4 mg/m<sup>3</sup>) C 0.2 ppm (0.8 mg/m<sup>3</sup>) [15-minute]  
OSHA PEL : TWA 0.1 ppm (0.4 mg/m<sup>3</sup>)

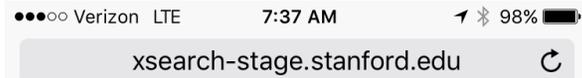
**Physical Description** Colorless gas with a suffocating odor like musty hay. [Note: A fuming liquid below 47°F. Shipped as a liquefied compressed gas.]

MW: 98.9	BP: 47°F	FRZ: -198°F	Sol: Slight	VP: 1.6 atm	IP: 11.55 eV
Sp.Gr: 1.43 (Liquid at 32°F)	Fl.P: NA	UEL: NA	LEL: NA	RGasD: 3.48	

Nonflammable Gas

**Incompatibilities & Reactivities** Moisture, alkalis, ammonia, alcohols, copper [Note: Reacts slowly in water to form hydrochloric acid & carbon dioxide.]

**Exposure Routes** inhalation, skin and/or eye contact (liquid)



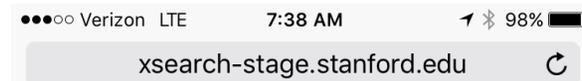
Phosgene Search

Navigation icons: Grid, Filter, Sort, Refresh, Share, Home, Menu

➔ Websites

<<< < 1 2 3 > >>>

- Results 1 - 20 of 59
- [Phosgene \(COCl<sub>2</sub>\)](#)   
Phosgene (COCl<sub>2</sub>). characteristics: colorless, h  
odor of mowed hay. symptoms of exposure:  
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... P095, 75-44-5, Carbonic dichloride, **Phosger**  
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e-EROS : Encyclopedia of Reagents for Organic  
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Method 1: From Phosgene Phosgene is the  
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Sartori, G.; Maggi, R.  
Science of Synthesis, (2005) **18**, 666.  
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[graceb@Stanford.edu](mailto:graceb@Stanford.edu)