

# Chemical Management Software

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and Lifecycle Management Workshop  
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Laboratory

# PNNLs Chemical Management System

- ▶ Custom-built ~ 1990
- ▶ Implemented ~ 1992
- ▶ Extensively modified since then
- ▶ Oracle-based
- ▶ Inventory management via barcode

# Purposes for the CMS

- ▶ Facility Use Agreement (FUA) Compliance – based on fire codes
- ▶ Hazard Communication Compliance
- ▶ Environmental Permitting
- ▶ Emergency Management
- ▶ QA
- ▶ Others ?

# Modules

- ▶ Ordering
- ▶ Inventory Record
- ▶ Pure Chemical and Product Properties
- ▶ Hazard Review
- ▶ Web Reporting
- ▶ MSDS – not linked to CMS
- ▶ Batch e-mailing – time sensitive chemicals, alerts, etc.

# Linkages to Other Systems

- ▶ Linked to purchase card system
- ▶ Linked to graphical map interface tool
- ▶ Other linkages
- ▶ Not linked to B-2-B purchasing
- ▶ Not linked to purchase order purchasing
- ▶ Not linked to waste system
- ▶ Not directly linked to MSDS system

# Chemical Management System

File Edit System Administration Chemical Orders Record Help Window

CMS© V 4.0 - Chemical Purchases. User: D3M116 (chem.prod.irm)

**Purchase Type**  
 Purchase Card  
 Purchase Requisition  
 Stores Order

Purchase ID:  (Query Only)  Template ?

Person who will appear on inventory record as the primary contact  
 Payroll #:  Name:   
 Phone:

**Deliver To** Name:  Building:   
 Payroll #:  Phone:  Room:

Inventory location (inventory records will show this building and room)  
 Building:  Room:

Inventory Control Group:  Date Reqd.:   Compressed Gas Order?

(Query Only)

Status Code:

P = printed  
 A = author released (if QA required)  
 R = fully released

Order Release Date:

Author Payroll #:

Shipping Instructions (appear on PCard printout)

Supplier Name:  Contact:   
 Address:  City:   
 State:  Zip:  Phone:  FAX:

**Charge Codes**

Number	% Split

**Purchase Items**

Item No.	Chem Item?	Chemical / Product name	Manufacturer Name	Catalog Item #	Uni Order
<input checked="" type="checkbox"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

CMS V 4.0 - Chemical Inventory ( Detail ). User: D3M116 ( chem.prod.irm )

Order    Unreleased Orders    Inventory ( Detail )    Inventory ( List )

Find    Prev.    Next    New    Delete    Clear    Save    MSDS    CMS Home Pg

Chemical Name **LITHIUM BOROHYDRIDE**    Static Inventory? **N**

Container ID # (Barcode #) 248124    Bldg. # EMSL    Room # 1430    On Order? **N**

Location Desc.    Query Only    Order # 11347554    Item # 002

CAS Number 16949-15-8    PNNL Chemical # 24366    MSDS Identification #

	Value	Unit			
Container Size	10	G	Acquisition Date	04/12/2006	Cost Code D7E52
Amt. in Container	10	G	Expiration Date (mm/yyyy)		Mfr # 2020
Concentration	95	PCT	Last Inventoried	03/19/2007	

Mr. Name SIGMA-ALDRICH    Mr. Catalog # 22,235-6    Storage Type Code

Primary Contact 3C733    Inv. Control Group    Project 90001    Lot #

[View Only](#)    Name Linehan, John C    Phone 375-3983

Comment     Available for Redistribution?    Delete

CMS© V4.0 - Pure Chemical Names, Properties & Hazard Groups Administration

Order    Unreleased Orders    Inventory ( Detail )    Inventory ( List )

Find    Prev.    Next    New    Delete    Clear    Clear All    Save    MSDS    CMS Home Pg

Chemical Name	Chemical #	Preferred Name or Synonym
LITHIUM TETRAHYDROBORATE	9000588	P
LITHIUM BOROXYDRIDE	9000588	S

Chemical # 9000588    CAS Number 16949-15-8    Molecular Weight 21.78

Physical State S    Density (gm/cc) .666    LD50 Oral Qty

TPQ    Lbs.    Threshold Qty    Lbs.    LC50 Inhalation Qty

Comment    Reviewed Y    LD50 Skin Qty

[View Only](#)    Air Compliance Information for Pure Chemical (if applicable)

Status    Approved by

Chemical Group Code	Chemical Group Description	Concentration Greater Than %	Concentration Up to %
FS	FLAMMABLE SOLIDS		
WRS2	WATER-REACTIVE SOLIDS - CLASS 2		
X2	CORROSIVE SOLIDS		



# CMS

Chemical Management System



New to CMS?

- Reports**  
[Inventory Report](#)  
[Other Reports](#)
- Tools**  
[CMS Tool](#)
- Assistance**  
[New User Help](#)  
[CMS Contacts](#)
- Basic Pages**  
[CMS Home](#)  
[Preferences](#)

## References

- ### MSDS
- [OHS](#)
  - [Image Wave](#)
  - [Offsite](#)

- ### SBMS
- [Chemicals](#)
  - [Chemical Hygiene](#)
  - [Data Access](#)

- ### IOPS
- [Request Chemicals](#)

- ### ChemAgain
- [Search](#)

- ### Tool Help
- [User Procedures](#)
  - [User Guide](#)

## Introduction

The Laboratory-wide Chemical Management System provides an effective way to track chemicals, ensure that safety and health information for each individual chemical in a given inventory is readily available and up-to-date, and to furnish an overall chemical management system. The procedures, users guide, and software are available electronically through a centralized system. The User Guide describes the practical applications of CMS

Staff who order and inventory chemicals must use the CMS software. The CMS User Procedures describes the required procedure for accessing and using the system. For more information about acquisition, use, handling, and storage of chemicals, see the Working With Chemicals subject area.

## Reports

- |  |   |                         |   |
|--|---|-------------------------|---|
| <a href="#">Building Limit Inventory</a> | <a href="#">Chemical Usage Administrative</a> | <a href="#">General</a> | <a href="#">Training Related Air Compliance</a> |
|--|---|-------------------------|---|
- [CMS Inventory](#)
  - [Chemicals Available for Redistribution](#)
  - [CMS Chemical Group Inventory](#)
  - [CMS Hazard Group Inventory](#)
  - [Chemicals by Hazard Group](#)
  - [CMS Threshold Quantity Inventory](#)
  - [CMS...](#)

## Reports

- Building Limit
- Chemical Usage
- General
- Training Related
- Inventory
- Administrative
- Air Compliance

- [CMS Inventory](#)
- [Chemicals Available for Redistribution](#)
- [CMS Chemical Group Inventory](#)
- [CMS Hazard Group Inventory](#)
- [Chemicals by Hazard Group](#)
- [CMS Threshold Quantity Inventory](#)
- [CMS Reportable Quantity Inventory](#)
- [CMS Inventory by Physical State](#)
- [CMS Bar Code Inventory History](#)
- [Expired Chemical Inventory](#)
- [Expired Chemical Inventory \(Role Based\)](#)
- [Toxic Air Pollutants Inventory](#)
- [APEL Summary Chemical Inventory by Group](#)
- [Building Reportable Quantity Inventory](#)
- [Chemical Inventory by Meta Group or Chemical Group](#)
- [Chemical Inventory with 300 Area Pre-empt](#)
- [Chemical Inventory Transaction Status](#)
- [Chemical Inventory Exception Listing](#)
- [CMS Immediate Precursor \(IP\) Inventory Listing](#)
- [Meta Group - Chemical Groups](#)
- [RPL Summary Chemical Inventory by Group](#)
- [CMS TQ & TPQ Chemicals Inventory](#)
- [300 Area FUA Quantity by Primary Contact](#)

Edit View Favorites Tools Help

Back Search Favorites

Address: <http://cms.pnl.gov/XMLReportInput.aspx?XMLFILE=InventoryReport.xml>

File Go Bookmarks Popups okay Check AutoLink AutoFill Send to Settings

**Search by:**

- Chemical Name
- CAS Number (basically pure products)
- Chem Number(s)
- CAS Number (any product containing the pure chemical constituent identified by the CAS number you enter)

**Chemical Name, CAS No, or Chem No(s):**

**Primary User Emplid No:**

**Organization Code:**

**Inv. Control Group:**

**Building:**

**Room No:**

**Location:**

**Select:**

- All
- On Order Items
- Static Items

**Display MSDS:**

- No
- Yes

**Summation Units:**

Edit View Favorites Tools Help

Back Search Favorites

Address: <http://cms.pnl.gov/XMLReportOutput.aspx?XMLFile=InventoryReport.xml>

Go Bookmarks Popups okay Check AutoLink AutoFill Send to Settings

## Inventory Report

CMS Inventory Listing

(restricted items not shown except to owner or admin.)

Export to Excel

Building	Room	Cntnr No.	Chemical Name	Conc.	Location	CAS No.	Quantity	LID	Contact Name	Phone No.	Chem No.
EMSL	1310	242466	LITHIUM BOROHYDRIDE	2.0 M		16949-15-8	100.00 ML	02/06	MG Warner	509/376-3804	24366
EMSL	1430	248124	LITHIUM BOROHYDRIDE	95.0 PCT		16949-15-8	10.00 G	03/07	JC Linehan	509/375-3983	24366
PSL	1520	249953	LITHIUM BOROHYDRIDE	2.0 MGB		16949-15-8	100.00 ML	04/06	S Autrey	509/375-3792	24366
PSL	1611	283701	LITHIUM BOROHYDRIDE	95.0 PCT		16949-15-8	50.00 G	04/07	L Li	509/375-2572	24366
PSL	1615	8655	LITHIUM BOROHYDRIDE		FC	16949-15-8	10.00 G	04/06	MA Lilga	509/375-4354	24366

Number of containers is 5, Totalling 0.59 LB

Export to Excel

Format last modified 07/25/2005. Send questions or comments to the [CMS Support Team](#).

Edit View Favorites Tools Help

Back [Navigation Icons] Search Favorites [Navigation Icons]

Address: <http://cms.pnl.gov/XMLReportOutput.aspx?XMLFile=ChemNamesPropsHazards.xml&HTMLOnly=True>

Go [Navigation Icons] Bookmarks Popups okay Check AutoLink AutoFill Send to Settings

Names & Synonyms	Preferred/Synonym
LITHIUM TETRAHYDROBORATE	P
LITHIUM BOROHYDRIDE	S

Chem No.	CAS No.	Molecular Weight
24366	16949-15-8	
Physical State	Density (gm/cc)	LD50 Oral Rat (mg/kg)
S		
Conc.Reqd?	MSDS No.	LC50 Inhalation RAT (ppm)
N		
TPQ (lbs)	Threshold Qty (lbs)	Comment

Constituent Name	Pure Chem No.	CAS No.	PCT of Product*	Primary?
LITHIUM TETRAHYDROBORATE	9000588	16949-15-8	100.000	Y

0.000 displayed for constituents less than .0005%.

Group ID	Hazard Group Name	Conc. > %	Conc. Up to %
K2	CORROSIVE SOLIDS	0.0	0.0
F5	FLAMMABLE SOLIDS	0.0	0.0
WRS2	WATER-REACTIVE SOLIDS - CLASS 2	0.0	0.0

CMS© V 4.0 - Product Names, Properties & Hazard Groups Administration. User: D3M116 (chem.prod.i)

Order    Unreleased Orders    Inventory ( Detail )    Inventory ( List )

Find    Prev.    Next    New    Delete    Clear    Clear All    Save    MSDS    CMS Home Pg

Product Name	Preferred Name or Synonym	Product #
WINDEX	P	45890
WINDEX GLASS CLEANER	S	45890

Product # 45890    Physical State L    Concentration Req'd. N    Molecular Weight

Comment    Density (gm/cc)    Periodicity    Primary CAS #

Admin. Review     Fire Review     Ind. Hygiene Review     Auto. System Review

Manufacturer #	Manufacturer Name	Image Wave MSDS #
1956	SC JOHNSON	35037

Pure Chemical Name / Constituent	Pure Chemical #	CAS Number	PCT of Product	Primary Constituent?
ISOBUTANE	9007557	75-28-5	3	<input type="checkbox"/>
2-BUTOXYETHANOL	9002793	111-76-2	5	<input type="checkbox"/>
PROPANE	9004163	74-98-6	1	<input type="checkbox"/>

Chemical Group Code	Chemical Group Description	Concentration Greater Than %	Concentration Up To %
GLYET	GLYCOL ETHERS		

# Entered/Exempted Items

- ▶ Required entry: anything with chemical hazard.
- ▶ Static inventories allowed.
- ▶ Not required to be entered in CMS:
  - | Nonhazardous items (after review)
  - | Biological agents (not biotoxins, which are entered)
  - | Office supplies used in normal consumer quantities
  - | Personal items for personal use (hair spray, etc.)
  - | Articles
  - | Building structural materials
  - | Inert gases
  - | Other items exempted on a case-by-case process upon review.

# Issues....and Into the Future

## ▶ Major issues:

- | Migrate or replace software by 2010
- | Define functional requirements

## ▶ The future:

- | Start clean/stay clean in new facilities
- | Integrated asset management: are chemicals assets?
- | Drive towards tighter management of chemicals will affect policy, software requirements
- | Significant laboratory interest in external CMS provider, perhaps to include software. Planning FY 2008 pilot project if funding available.