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National Nuclear Security Administration

International Nonproliferation Export Control Program (INECP)

Chemicals in CIT

Chemical identification strategies and the Chemical Cross-Reference

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Chemicals Module Objective

- **Increase familiarity with controlled chemicals and resources to facilitate their identification in shipments**

The Chemicals CIT module introduces numerical codes helpful for chemical identification, followed by an overview of controlled chemicals for awareness purposes.

CIT Strategy on Chemicals

- The focus of CIT is visual identification, but chemicals cannot be definitively identified by their physical appearance
- Often multiple chemical names are valid for a single substance, making reliance on names potentially misleading
- Therefore, the CIT Chemicals module focuses on identifying codes that can assist with identification
  - "Nameplate" concept
  - Still discuss appearance and packaging for completeness
  - Keep in mind potential for chemical sampling and analysis by laboratory personnel

Useful Markings for Identifying Chemicals

- **Chemical Name: Control list name identifies chemical, but can have many valid synonyms**
  - Thiodiglycol = Thiodiethanol = 2-Hydroxyethyl sulfide = …

- **CAS #: Chemical Abstracts Service registry number - Unique**
  - (XXXXX)XX-XX-X, where X is any number 0-9. Thiodiglycol = 111-48-8
  - Unambiguous identifier; millions of registered chemicals

- **EC # (EINECS): European registry - Unique**
  - YYY-YYY-Y, where Y is any number 0-9. Thiodiglycol = 203-874-3

- **UN #: United Nations number for hazardous chemicals**
  - UN ZZZZ or ZZZZ, where Z is any number 0-9. Thiodiglycol = UN 3334
  - Not always unique (same UN number can apply to multiple chemicals; thiodiglycol number is not unique)

Chemical Abstracts Service and the CAS Registry

- **CAS = Chemical Abstracts Service**
  - Division of the American Chemical Society
  - Provides data products for chemical research and identification
- **CAS Registry**
  - Currently has records for over 52 million organic and inorganic substances
  - Updated daily (~12,000 new substances per day)
  - Each record assigned a CAS Registry Number

"When a chemical substance, newly encountered in the literature, is processed by CAS, its molecular structure diagram, systematic chemical name, molecular formula, and other identifying information are added to the Registry and it is assigned a unique CAS Registry Number."

CAS website: http://www.cas.org

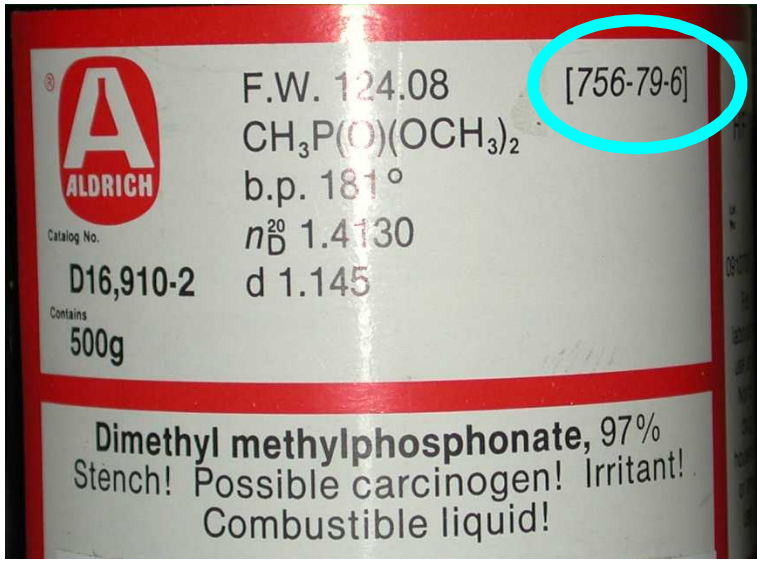
CAS Registry Numbers (CAS #s or CAS RNs)

- **Features of CAS #s**
  - Unique numeric identifiers: help circumvent ambiguity of multiple chemical names
  - No chemical significance
  - US origin, but used internationally
- **Format**
  - Three parts separated by hyphens, up to nine digits total
  - Last digit is a “check digit” for validity and uniqueness (http://www.cas.org/expertise/cascontent/registry/checkdig.html)
- **Included with chemical names in the AG precursor control list and many national control lists**

(XXXXX)XX – XX – X

CAS Numbers and Chemical Shipments

- **CAS#s are typically found on inner packaging**
- **Container label**
  - Look for pattern of digits: (XXXXX)XX-XX-X
- **Paperwork**
  - Material Safety Data Sheets
  - Specification/Quality Assurance Sheets
- **Online chemical search engines can help find CAS#s given chemical name or vice versa**



Product Name	Dichloromethylphosphine
Product Number	46,684-0
CAS Number	676-83-5
Molecular Formula	CH_3Cl_2P
Molecular Weight	116.9

TEST	SPECIFICATION
APPEARANCE	COLORLESS LIQUID
INFRARED SPECTRUM	CONFORMS TO STRUCTURE.
PROTON NMR SPECTRUM	CONFORMS TO STRUCTURE.
PHOSPHORUS 31 NMR	CONFORMS TO STRUCTURE.

CAS Number References/Resources

Free (besides Google)	
Chemistry WebBook (NIST)	webbook.nist.gov/chemistry
Chemical companies	Numerous
Sigma-Aldrich	www.sigmaaldrich.com
Fisher Scientific Product Search	www.fishersci.com
Pfaltz & Bauer	www.pfaltzandbauer.com
Supplier databases/search engines	Numerous
ChemExper	www.chemexper.com
BuyersGuideChem	www.buyersguidechem.de
OPCW Scheduled Chemicals Database (free registration required; CWC Schedules only)	https://apps.opcw.org/cas/
Paid subscription	
CAS Databases	www.cas.org/casdb.html

Searches on CAS#s are available through these resources

UN Model Regulations

- **UN Recommendations on the Transport of Dangerous Goods**
  - Known as the "Model Regulations"
  - Developed by the United Nations Economic and Social Council's Committee of Experts on the Transport of Dangerous Goods
  - Serve as guidelines for dangerous goods shipping regulations of governments and international organizations
  - **Origin of UN Numbers and associated labeling practices**
    - ***Part 3: Dangerous Goods List (UN Numbers)***
    - ***Part 5: Consignment Procedures***

"The Model Regulations aim at presenting a basic scheme of provisions that will allow uniform development of national and international regulations governing the various modes of transport; yet they remain flexible enough to accommodate any special requirements that might have to be met."

— Recommendations on the Transport of Dangerous Goods

UN Numbers

- Code assigned to a **hazardous** substance or article under the United Nations System
- Found in the Dangerous Goods List of the UN “Model Regulations”
- Properties
  - Four digits long
  - May represent a specific chemical or a category of hazardous chemicals
    - *1809 = Phosphorus trichloride*
    - *1993 = Flammable liquid, not otherwise specified*
- General categories might include controlled chemicals, but you will need to find more information on the substance to determine the chemical’s identity

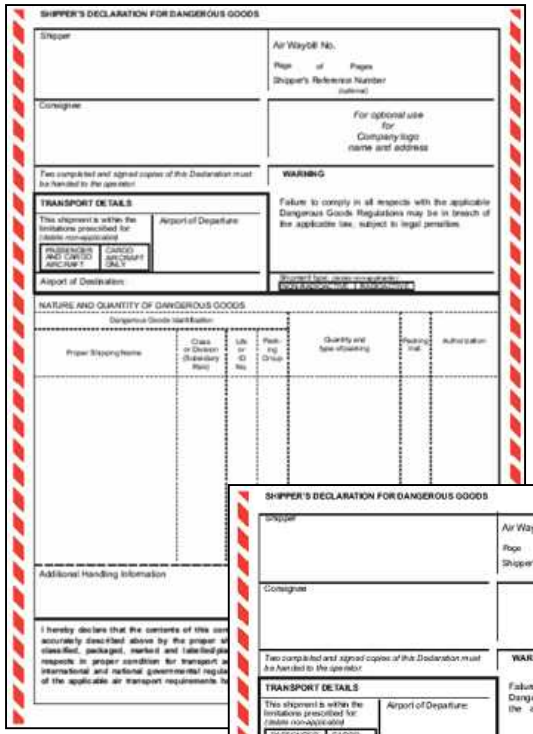
UN number and diamond label arrangements (1203 is gasoline)

Proper Shipping Name (PSN)

- **Name of the hazardous substance in the UN Dangerous Goods List (all capital letters)**
- **Use in shipping**
  - Should be included on packaging and hazardous goods shipping documents near UN number
  - Might be included on “transport units”
- **Generic or “not otherwise specified” PSNs**
  - In general, must be supplemented by a technical name
  - Trade names are prohibited
  - Example: UN 1993 FLAMMABLE LIQUID, N.O.S. (dimethyl phosphite)

UN Numbers and Documentation

- **UN Numbers and PSNs are required on hazardous goods shipping documents**
  - IATA
  - IMO
  - Multimodal
  - Etc.
- **First column: UN number or PSN**
  - UN number first preferred



NATURE AND QUANTITY OF DANGEROUS GOODS			
Dangerous Goods Identification			
UN or ID No.	Proper Shipping Name	Class or Division (Subsidiary Risk)	Packing Group
UN 1385	SODIUM SULPHIDE, ANHYDROUS	4.2	II

UN Number References/Resources

- **UN Model Regulations, 16th Revised Edition (2009)**
  - www.unece.org/trans/danger/publi/unrec/rev16/16files_e.html
- **YOW Canada Dangerous Goods Info Search**
  - www.yowcanada.com/DG-Search.asp
- **2008 Emergency Response Guidebook**
  - phmsa.dot.gov/hazmat/library/erg
- **Labelmaster PSN (Proper Shipping Name) Wizard**
  - Makes label associated with a UN Number
  - www.labelmaster.com/resources/PSNWizard
- **Swedish Coast Guard website**
  - Overview of dangerous goods transport labeling
  - www.coastguard.se/ra/volume2/annexes/annex6.htm
- **IATA dangerous goods shipping declarations**
  - www.iata.org/whatwedo/cargo/dangerous_goods/download.htm

Other Chemical Identification Codes: EC and Control List Numbers

- **EC Numbers: Another unique code**
  - Formerly known as EINECS Numbers
    - *European INventory of Existing Chemical Substances*
    - *Chemicals on the market in Europe between January 1, 1971 and September 18, 1981*
  - Format: YYY-YYY-Y
  - Registry contains 100,196 chemicals
  - Found at European Chemicals Bureau website: http://ecb.jrc.ec.europa.eu/esis/
- **Control List Numbers**
  - US CIT presentations use codes from EU Dual Use List
    - *Council Regulation (EC) 394/2006 of February 27, 2006*
    - *trade.ec.europa.eu/doclib/docs/2006/march/tradoc_127868.pdf*
  - Institutionalized presentations should include codes from national legislation

Other Chemical Identification Codes: Harmonized (Tariff) System Numbers

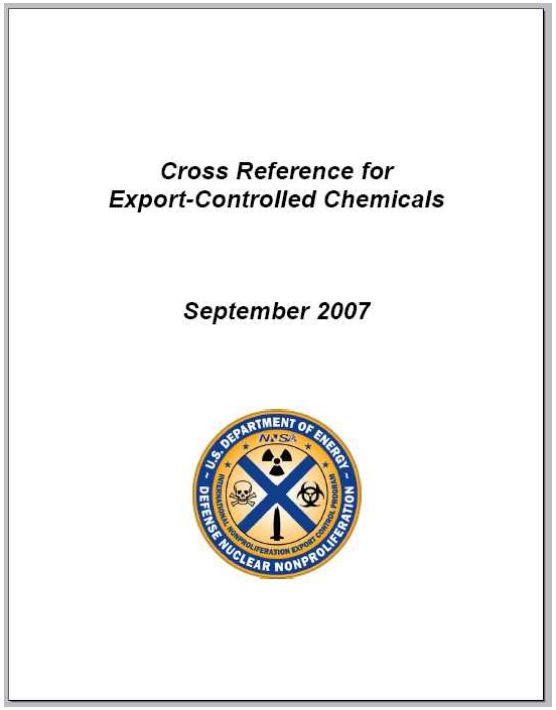
- **Included at the six-digit level on CIT slides**
- **Advantages**
  - Familiar to Customs officers
  - Harmonized internationally to six digits
    - *Example: WCO recommendations on CWC Scheduled chemicals (www.wcoomd.org/files/1. Public files/PDFandDocuments/HarmonizedSystem/HS Recommendations/HS_reco_june2009_EN.pdf)*
- **Disadvantages**
  - Six-digit numbers are too general for definitive identification
  - Use of six-digit numbers without recognizing this can mislead students
- **Some countries have assigned eight or ten digit tariff numbers specific to CW precursors**
  - Example: Australia (www.dfat.gov.au/cwco/cd_rom_imp_exp_chem.html)
  - Extending number of digits in CIT modules may be worthwhile for CIT indigenization in this case

Material Safety Data Sheets (MSDS)

- **MSDS provide information for employers, employees, and response personnel who could be exposed to chemical hazards**
- **Typical MSDS information**
  - **Manufacturer and emergency contact information**
  - **Chemical name and synonyms**
  - **CAS #s**
  - Physical data
  - Toxicity information
  - First aid and recommended protective equipment
  - Storage and disposal information
  - Spill/accident procedures
  - **Transportation regulations (UN numbers)**
- **Format is not uniform for all companies**

MSDS HyperGlossary Links: http://www.ilpi.com/msds/index.html

Using the Cross Reference for Export-Controlled Chemicals



- **Assists with determining whether or not a chemical is export controlled**
- **Organized by 8 means of identification, including**
  - Names w synonyms
  - CAS#, UN, HS

Export-Controlled Chemicals
Cross Reference

This booklet is intended to assist in determining whether or not a chemical qualifies for export control under any of several multilateral export control regimes. It lists several AG, NSG, MTCR, and CWC chemicals, organized by eight means of identification.[1]

[1] Due to the presence of categories of chemicals, rather than specific chemicals, in some regime lists (e.g., the CWC Schedules), this booklet does not include every possible controlled chemical. However, it includes all AG chemicals and a substantial number of those from other regimes. Wassenaar Arrangement chemicals are listed only to the extent that they overlap with chemicals listed in the other regimes.

2

Chemical Cross-Reference Handout

- **The *Cross-Reference of Controlled Chemicals* handout organizes controlled chemicals by**
  - Control list chemical names and synonyms
  - Codes: CAS, EC, EU Control List, US Control List, and six-digit Harmonized System numbers
  - UN numbers
    - *Number and PSN for controlled chemicals with unique UN#*
    - *Some examples of general categories that can include controlled chemicals*
- **The handout does NOT include every possible controlled chemical. However, it does include**
  - All AG CW precursors (63 precursors as of November 2004)
  - Selection of
    - *CWC Scheduled chemicals not on the AG list*
    - *NSG chemicals*
    - *MTCR chemicals*