What Chemical is That?

Picture this hypothetical event. Responders enter a vacant/abandoned building and discover a room containing many different chemicals stored in bottles and packages on shelves. There are also a few 55-gallon drums, 5 and 10 gallon containers, and sacks of various materials on the floor. The containers and sacks appear to have labels, but some labels are obscure or have minimal identification. There is no obvious indication of illegal activity other than possible improper storage of incompatible chemicals in the room and possible violation of community-right-to-know regulations. The owner(s) of the chemicals are unknown or can't be located. The area is secured, and specialists are brought in to try to figure out what is there in order that a plan for removal and safe disposal may be developed. Caution must be exercised by anyone entering the area as some chemicals can form explosive peroxides or undergo destructive polymerization reactions rupturing the container on long-term storage, and it is not yet known what chemicals are in the containers. What chemicals are in the room, and what are the hazards?

The American Chemical Society recognizes about 34 million different chemicals, at least this is the number of chemicals that have been assigned chemical abstract service (CAS) registry numbers to date. Many of these chemicals are known by different names (e.g. dichloromethane and methylene dichloride are the same thing); some chemicals can have say 20 or even more than 40 names. Commercial product formulations are usually mixtures of different chemicals. With so many chemicals and product formulations, sometimes two different chemicals or mixtures are known by the same name. This creates confusion for someone trying to figure out, "what chemical is that?"

We will look at some tips on locating and identifying obscure chemical names, how chemicals are named, and some reference sources for finding Material Safety Data Sheets.

Chemical Abstracts Service Registry Numbers

The Chemical Abstract Service (CAS), a division of the American Chemical Society, assigns a unique identifying number for every chemical that has been described in the literature. To date, the total CAS numbers that have been added are about 34 million for chemicals and 60 million for biological sequences. About 50,000 new numbers are added each week. The intent is to provide a unique identifier as chemicals can be called by many different names. The CAS number does not provide information as to the concentration of chemical or its manufacturer.

Fortunately, for the first responder and others interested in public safety, only a few thousand chemicals are of concern. Perhaps another 10,000 or 20,000 chemicals might appear on some lists. The PEAC tool lists about 130,000 entries counting synonyms and shipping names.

A CAS registry number is separated by hyphens into three parts, e.g. 630-08-0 for "Carbon monoxide". The numbers are assigned in increasing order in which they appear in the literature or described by researchers (at least since 1957) and do not have any inherent meaning as to chemical structure or use. The first sequence of numbers (e.g. "630" in 630-08-0) can have up to 8 digits, the second sequence always has 2 digits, and the last sequence always consists of a single digit which is used as a summation check. This last digit is a check against someone accidentally entering a wrong number, a useful tool for any computer check of data bases containing CAS#s. To use this check, the last digit in the second sequence is multiplied by 1, the next digit to the left is multiplied by 2, the next digit to the left is multiplied by 3, etc., and results summed. The last digit in the summation should be equal to the single digit in the third sequence. For example, sulfur monochloride has a CAS# = 10025-67-9. 7*1 + 6*2 + 5*3 + 2*4 + 0*5 + 0*6 + 1*7 = 49. The last digit of the summation is "9" and this is the same as the digit in the third sequence.

The CAS# is a very useful tool when comparing data bases as often the chemicals in different data bases may use different chemical names. This makes it especially useful for government and regulations listing chemicals.

If the only information known about a chemical is its CAS#, often the chemical name and sometimes even a Material Safety Data Sheet (MSDS) can be located on the Internet by typing in the CAS# in a computer search engine such as Google. When using a computer search engine, be sure to type in quotes e.g. "10025-67-9" and "CAS" or otherwise the search engine will pull up dates, street addresses, and other junk which have no relationship to the CAS#.

While not an Occupational Safety and Health Administration (OSHA) requirement, the MSDS often contains the CAS number. If the material is a mixture of different chemicals, the CAS number for each component may be listed on the MSDS for the mixture.

When using CAS numbers, each isomer of a molecule will have a unique CAS# and sometimes mixtures of isomers or an unspecified isomer will have a separate CAS#. For example, xylene(mixed isomers) has a CAS# = 1330-20-7; the individual isomers are m-xylene which has a CAS#=108-38-3, p-xylene has a CAS#= 106-42-3, and o-xylene has a CAS#=95-47-6. Sometimes m-xylene is referred to as meta-xylene, p-xylene as para-xylene, and o-xylene as ortho-xylene. All have the same chemical formula C_8H_{10} . But each isomer has different melting and boiling points, different flash points, and different hazard considerations. Therefore from a hazard point of view the entries should be kept separate.

When doing a data base search by CAS#, all derivatives of the chemical should be included. For example, the drug "meth" can refer to "methamphetamine" which has a CAS number of 537-46-2 or "methamphetamine hydrochloride" which has a CAS number of 51-57-0. Methamphetamine hydrochloride is the usual form of the drug encountered on the street, and is usually what is called "meth", "speed", "ice", "crystal

meth", and many other names. The Merch Index, published by Merch & Company, Whitehouse Station, N.J. is a good reference source for the various drug derivatives and their CAS numbers.

Sometimes mixtures of individual chemicals are assigned their own CAS number if they fall into a particular category. Petroleum refinery cuts are an example. Table 1 lists a few example listings for refinery cuts, which were taken from a U.S. government regulations list of chemicals (Code of Federal Regulations, Title 40 Part 710 subpart C on inventory reporting requirements, exempt chemicals), available at http://edocket.access.gpo.gov/cfr 2004/julqtr/40cfr710.46.htm).

 Table 1 Example CAS Numbers for Refinery Cuts (see website for a much longer list)
 63231-60-7 Paraffin waxes and hydrocarbon waxes, microcryst. 64741-41-9 Naphtha (petroleum), heavy straight-run 64741-42-0 Naphtha (petroleum), full-range straight-run 64741-43-1 Gas oils (petroleum), straight-run 64741-44-2 Distillates (petroleum), straight-run middle 64741-45-3 Residues (petroleum), atm. tower 64741-46-4 Naphtha (petroleum), light straight-run 64741-47-5 Natural gas condensates (petroleum) 64741-49-7 Condensates (petroleum), vacuum tower 64741-50-0 Distillates (petroleum), light paraffinic 64741-51-1 Distillates (petroleum), heavy paraffinic 64741-52-2 Distillates (petroleum), light naphthenic 64741-53-3 Distillates (petroleum), heavy naphthenic 64741-54-4 Naphtha (petroleum), heavy catalytic cracked 64741-55-5 Naphtha (petroleum), light catalytic cracked 64741-56-6 Residues (petroleum), vacuum 64741-57-7 Gas oils (petroleum), heavy vacuum 64741-58-8 Gas oils (petroleum), light vacuum 64741-59-9 Distillates (petroleum), light catalytic cracked 64741-60-2 Distillates (petroleum), intermediate catalytic cracked 64741-61-3 Distillates (petroleum), heavy catalytic cracked 64741-62-4 Clarified oils (petroleum), catalytic cracked 64741-63-5 Naphtha (petroleum), light catalytic reformed 64741-64-6 Naphtha (petroleum), full-range alkylate 64741-65-7 Naphtha (petroleum), heavy alkylate 64741-66-8 Naphtha (petroleum), light alkylate

64741-67-9 Residues (petroleum), catalytic reformer fractionator

64741-68-0 Naphtha (petroleum), heavy catalytic reformed
64741-69-1 Naphtha (petroleum), light hydrocracked
64741-70-4 Naphtha (petroleum), isomerization
64741-73-7 Distillates (petroleum), alkylate
64741-74-8 Naphtha (petroleum), light thermal cracked
64741-75-9 Residues (petroleum), hydrocracked

Each refinery cuts are mixtures of many different individual chemicals. The individual chemicals (hexane, heptane, ethylene, octane, etc.) have their individual CAS numbers and the refinery cut also has its CAS number.

Gasoline is a complex mixture of approximately 230 different chemicals. It includes various refinery cuts, possibly ethyl benzene, possibly ethyl alcohol, and various additives. Natural gasoline has a CAS number of 8006-61-9, but gasoline as marketed today also has many additives some of which are also listed with their CAS#s (example specification at <u>http://www.hazard.com/msds/f2/brg/brggt.html</u>, several CAS numbers listed including 8006-61-9). The listing can vary depending upon the formulation. Sometimes the CAS number 8006-61-9 will not appear at all but instead the CAS number for other refinery cuts plus additives, and not all components will be listed.

The American Chemical Society, Columbus Ohio, maintains a CAS registry where clients can search for and confirm CAS numbers for millions of substances. The service is not free. Details are at the website,

http://www.cas.org/products/client/lookup/index.html.

Chemical Names

Individual chemicals can be called by many different names. For example, let us look at the pesticide malathion which has a CAS number of 121-75-5. It is a widely used to control mosquitoes, certain animal external parasites, lice, flies, and sucking and chewing insects. There are concerns on toxicity to wildlife, especially honeybees. If the government National Institute of Standards and Technology (NIST) website is checked (see http://webbook.nist.gov/cgi/cbook.cgi?ID=121-75-5&Units=SI), a long list of alternative names including brand or trade names can be pulled up:

Other names for malathion: Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester; Succinic acid, mercapto-, diethyl ester, S-ester with O,O-dimethyl phosphorodithioate; [(Dimethoxyphosphinothioyl)thio]butanedioic acid, diethyl ester; American Cyanamid 4,049; Carbetox; Carbofos; Carbophos; Compound 4049; Cythion; Ethiolacar; Etiol; ENT 17,034; Fog 3; Fosfothion; Fosfotion; Fyfanon; Insecticide No. 4049; Karbofos; Malafor; Malamar 50; Malaspray; Malathion E50; Malathion LV Concentrate; Malatol; Mercaptosuccinic acid diethyl ester, S-ester with O,O-dimethyl phosphorothioate; Mercaptothion; Moscarda; O,O-Dimethyl S-(1,2-dicarbethoxyethyl) dithiophosphate; Oleophosphothion; Ortho Malathion; Phosphothion; Prioderm; S-[1,2-

Bis(carbethoxy)ethyl] O,O-dimethyl dithiophosphate; S-[1,2-Bis(ethoxycarbonyl)ethyl] O,O-dimethyl phosphorodithioate; Sadofos; Sadophos; Siptox I; Staeubol-Puder; Sumitox; SF 60; TM-4049; Zithiol; 8059HC; S-[1,2-Di(ethoxycarbonyl)ethyl] OOdimethyl phosphorodithioate; AC 26691; Carbethoxy malathion; Chemathion; Dicarboethoxyethyl O,O-dimethyl phosphorodithioate; Diethyl mercaptosuccinate, O,Odimethyl dithiophosphate, S-ester; Diethyl mercaptosuccinate, O,O-dimethyl phosphorodithioate; Diethyl mercaptosuccinate, O,O-dimethyl thiophosphate; Diethyl mercaptosuccinic acid, S-ester of O,O-dimethyl phosphorodithioate; Diethyl 2-(dimethoxyphosphinothioylthio)succinate; Dithiophosphate de O,O-dimethyle et de S-(1,2-dicarboethoxyethyle); Emmatos; Emmatos extra; Experimental insecticide 4049; Formal; Four thousand forty-nine; Kop-Thionkypfosmalacide; Malagran; Malakill; Malamar; Malaphos; Malathione; Malathon; Malation; Malatox; Malphos; MLT; NCI-C00215; O,O-Dimethyl dithiophosphate of diethyl mercaptosuccinate; O,O-Dimethyl S-(1,2-dicarbethoxyethyl) phosphorodithioate; O,O-Dimethyl S-(1,2-dicarbethoxyethyl) thiothionophosphate; O,O-Dimethyl S-1,2-di(ethoxycarbamyl)ethyl phosphorothioate; O,O-Dimethyl-S-1,2-dikarbetoxylethylditiofosfat; O,O-Dimethyldithiophosphate diethylmercaptosuccinate; S-(1,2-Bis(aethoxy-carbonyl)-aethyl)-O,O-dimethyldithiophasphat; S-(1,2-Bis(ethoxy-carbonyl)-ethyl)-O,O-dimethyl-dithiofosfaat; S-(1,2-Bis(etossi-carbonil)-etil)-O,O-dimetil-ditiofosfato; S-(1,2-Dicarbethoxyethyl) O,Odimethyl phosphorodithioate; S-1,2-Bis(ethoxycarbonyl)ethyl-O,O-dimethyl thiophosphate; Taskil; 1,2-D.(ethoxycarbonyl)dimethyl phosphorothiolothionate; 1,2-Di(ethoxycarbonyl)ethyl O,O-dimethyl phosphordithioates; Calmathion; Carbetovur; Celthion; Cimexan; Detmol MA; S-(1,2-Dicarbethoxyethyl) O,Odimethyldithiophosphate; 1,2-Di(ethoxycarbonyl)ethyl O,O-dimethyl phosphorodithioate; S-(1,2-Di(ethoxycarbonyl)ethyl) dimethyl phosphorothiolothionate; Diethyl (dimethoxyphosphinothioylthio) butanedioate; Diethyl (dimethoxyphosphinothioylthio)succinate; Diethyl mercaptosuccinate S-ester with O,Odimethylphosphorodithioate; Diethyl mercaptosuccinic acid O,O-dimethyl phosphorodithioate; O,O-Dimethyl S-1,2-di(ethoxycarbamyl)ethyl phosphorodithioate; O,O-Dwumetylo-S-1,2-bis(karboetoksyetylo)-dwutiofosforan; EL 4049; Externathion; Forthion; Fosfotion 550; Hilthion; Hilthion 25wdp; Kop-thion; Kypfos; Latka 4049; Malacide; Malaphele; Malasol; Malathiozoo; Maldison; Malmed; Maltox; Maltox MLT: Mercaptosuccinic acid diethyl ester; Mercaptotion; NA 2783; OMS 1; Sadofos 30; TAK; Vegfru malatox; Vetiol; Mychel; Mycinol; Cleensheen; Derbac-M; Diethyl [(dimethoxyphosphinothoiyl)thio]butanedioate; Lice Rid; Malathion 60; o,o-Dimethyl-S-(1,2-di(ethoxycarbonyl)ethyl) phosphorodithioate; Organoderm; Suleo-M; Diethyl 2-[(dimethoxyphosphorothioyl)sulfanyl]succinate.

Brand or trade names for malathion products can have other ingredients in the formulation besides malathion.

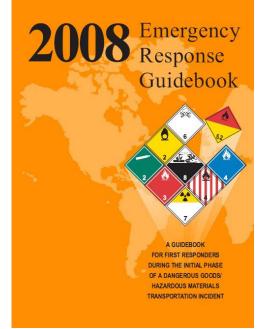
Synonyms and brand names for malathion are also listed at the U.S. National Library of Medicine TOXNET website, at <u>http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~obuoMn:1</u>. Click on "synonyms".

The point is that alternative names for chemicals can be complex and long.

Question: With the many different chemicals, and many of the chemicals are known by different names, is there any chance that the same name can be used for two different chemicals? **Answer**: Unfortunately yes, although not very often. People don't like to use long names because they are hard to remember and they must be entered into a computer search tool exactly right. Therefore they will invent short names that are easy to remember. The military likes to use acronyms. When short names or acronyms are invented, there is a good chance that the same name will be used for two different chemicals. For example, "H" can mean either hydrogen or mustard gas, two unrelated materials. "HD" can mean mustard gas, distilled; "HD" can also mean hydrogen deuteride. "DDE" links up to several different chemicals with different CAS numbers. Rarely brand or trade names might be used more than once; we have seen a few instances where names for a pesticide formulation also have been used for a flavoring agent (an unrelated chemical), or a drug used in medicine.

Shipping Names for Dangerous Goods/Hazardous Materials

Most responders in North America are familiar with the 2008 Emergency Response Guidebook (2008 ERG) which lists dangerous goods/hazardous materials. The ERG is updated every four years. Each entry is proceeded by a 4digit ID number and the name of the material, e.g. "1017" for chlorine, "1203" for gasoline. The ERG contains a section where the names of the materials are listed alphabetically and linked to the 4-digit ID number and another section where the ID numbers are in numerical order and linked to the material. By regulation, the ID number appears on the container or transportation vessel identifying the material being shipped. An English copy of the 2008 ERG can be downloaded off the Internet at http://hazmat.dot.gov/pubs/erg/erg2008 eng.pdf. French and Spanish versions are also available.



The 4-digit ID Number on the containers is proceeded by the letters NA or UN, e.g. UN1993, NA1993, NA9163, UN1962. "UN" means that the ID Number is used internationally including the United States and Canada and "NA" is restricted to the United States and Canada only. UN numbers range from 0004 to about 3500, and most NA numbers range from 8000 to about 9500. For the very few situations where NA and UN uses the same number, there may be variations in the shipping name, e.g., NA1993 uses "Combustible liquid, n.o.s." and a laundry list of selected examples and UN1993 uses the simple name "Flammable Liquid, n.o.s.". The 2008 ERG does not make UN and NA distinctions, and both shipping names are listed.

Each ERG 4-Digit ID Number (whether UN or NA) is always linked to the same Guide Number for emergency response.

Looking through the 2008 ERG, there are a lot of gaps in the 4-digit numbering sequence. Old additions (1996, 2000, 2004) list some of the missing numbers, and there are new ID Number additions to the 2008 ERG, which do not appear in earlier editions. The 2008 ERG also does not list ordinance UN ID numbers running from 0004 to about 0505. The 2008 ERG UN Numbers follows the 15th edition of UN Recommendations on the Transport of Dangerous Goods published in 2007. Periodically the United Nations Transport of Dangerous Goods Subcommittee meet and update UN Recommendations (see "http://www.phmsa.dot.gov/hazmat/regs/international" for a notice of a December 2008 meeting on an upcoming 16^{th} edition). The changes in the ID numbers and shipping names are documented. When old 4-digit numbers are deleted, the materials/chemicals are shipped under different 4-digit designations. There is a trend to use category names representing a hazard rather than assigning a UN number to a particular chemical, for example, UN2888, shipping name "tert-Butyl peroxy-2-ethylhexanoate, not more than 50%, with phlegmatizer" is obsolete, and the chemical might be shipped under UN3115, with shipping name "Organic peroxide type D, liquid, temperature controlled". The United Nations Subcommittee only issues recommendations. It is up to the individual countries to codify the United Nations recommendations into regulations.

A copy of the 15th edition of the UN Recommendations on the Transport of Dangerous Goods (sometimes called the orange book) can be obtained commercially at <u>http://www.costha.com/publications1.htm#UN%20Orange%20Book</u>. A free source is available in pdf format at

http://www.unece.org/trans/danger/publi/unrec/rev15/15files_e.html. The UN numbers are assigned by the United Nations committee, Economic and Social Council Committee of Experts on the Transport of Dangerous Goods. A list of all the current UN numbers and shipping names in the 15th edition is available at

http://www.unece.org/trans/danger/publi/unrec/rev15/English/03E_Part3.pdf.

Each UN 4-Digit ID number is linked to a unique shipping name, but each country lists the shipping name in its own language. Also there may be variations on how the shipping name is listed between different countries that speak the same language. An example is the shipping name "Flammable Liquids, n.o.s." linked to UN1993. This is the way the shipping name is listed at the website list cited above. But the NA1993 shipping name is listed as "Combustible liquid, n.o.s. or Compounds, cleaning liquid or Compounds, tree killing liquid or Compounds, weed killing, liquid or Diesel fuel or Fuel oil (No. 1, 2, 4, 5, or 6) or Medicines, flammable, liquid, n.o.s. or Refrigerating machine". The 2008 ERG uses multiple separate listings for 1993 reflecting NA1993 and UN1993. All NA1993 and UN1993 listings have the same Guide Number 128 for

emergency response.

1993 **128** Combustible liquid, n.o.s.

1993 128 Compound, cleaning liquid(flammable)

1993 128 Compound, tree or weed killing, liquid (flammable)

1993 128 Diesel fuel

1993 128 Flammable liquid, n.o.s.

1993 128 Fuel oil

The multiple listings in the 2008 ERG leave the responder guessing as to what the entries have in common to fall under the umbrella "1993" until the Guide Number 128 - Flammable Liquids is referenced. To add to the confusion, the 2008 ERG also links 1202 to Diesel fuel and several other UN ID numbers to refrigerating machines. The answers can be resolved by referring to the 15^{th} edition of the United Nations document cited earlier.

There are many flammable (or combustible) liquids. Therefore many chemicals and product formulations appearing on Material Safety Data Sheets (MSDS) will be linked to UN1993 even though they are not specifically listed in the 2008 ERG.

The 2008 ERG lists a few selected chemicals linked to a UN ID Number even though the chemical name does not appear in the shipping name. The official shipping name for UN2810 is "Toxic liquid, organic, n.o.s." Under that heading, the 2008 ERG lists specific many specific examples of chemical warfare agents and other toxic organic compounds, plus variations of the shipping name: 2810 **153** Buzz

2810 153 BZ 2810 153 Compound, tree or weed killing, liquid (toxic) 2810 153 CS 2810 153 DC 2810 153 GA 2810 153 GB 2810 153 GD 2810 153 GF 2810 153 H 2810 153 HD 2810 153 HL 2810 153 HN-1 2810 153 HN-2 2810 153 HN-3 2810 153 L (Lewisite) 2810 153 Lewisite 2810 153 Mustard 2810 153 Mustard Lewisite 2810 153 Poison B, liquid, n.o.s. 2810 153 Poisonous liquid, n.o.s. 2810 153 Poisonous liquid, n.o.s. (Inhalation Hazard Zone A) 2810 153 Poisonous liquid, n.o.s. (Inhalation Hazard Zone B) 2810 153 Poisonous liquid, organic, n.o.s. 2810 153 Poisonous liquid, organic, n.o.s. (Inhalation Hazard Zone A) 2810 153 Poisonous liquid, organic, n.o.s. (Inhalation Hazard Zone B) 2810 153 Sarin 2810 153 Soman 2810 153 Tabun 2810 153 Thickened GD 2810 153 Toxic liquid, n.o.s. 2810 153 Toxic liquid, n.o.s. (Inhalation Hazard Zone A) 2810 153 Toxic liquid, n.o.s. (Inhalation Hazard Zone B) 2810 153 Toxic liquid, organic, n.o.s. 2810 153 Toxic liquid, organic, n.o.s. (Inhalation Hazard Zone A) 2810 153 Toxic liquid, organic, n.o.s. (Inhalation Hazard Zone B)

2810 **153** VX All UN2180 listings have the same Guide Number 153 for emergency response.

[Comment: There are legal issues on shipping or even possessing chemical warfare agents; the listing of UN2810 on a package with "Toxic liquid, organic, n.o.s" does not mean that someone can transport chemical warfare agents.]

The same chemical may be assigned different UN ID Numbers depending upon how it is packaged. An example are the pesticides. There are over 1000 pesticide chemicals and over 10,000 product or trade formulations recognized by the U.S. Environmental Protection Agency. Many of the toxic pesticides can be placed into various classes (table 2) and assigned UN ID numbers depending upon whether the particular chemical is formulated as a solid or a liquid, and if a liquid the degree of flammability based on flash point:

Pesticide Class	Solid,	Liquid,	Liquid, toxic,	Liquid,
	toxic	toxic	flammable	flammable, toxic
Arsenical pesticide	2759	2994	2993	2760
Benzoic derivative	2769	3004	3003	2770
pesticide				
Bipyridilium pesticide	2781	3016	3015	2782
Carbamate pesticide	2757	2992	2991	2758
Copper based pesticide	2775	3010	3009	2776
Coumarin derivative	3027	3026	3025	3024
pesticide				
Dithiocarbamate	2771	3006	3005	2772
pesticide				
Organochlorine	2761	2996	2995	2762
pesticide				
Organophosphorus	2783	3018	3017	2784
pesticide				
Organotin pesticide	2786	3020	3019	2787
Pesticide, n.o.s.	2588	2902	2903	3021
Phenoxyacetic acid	3345	3348	3347	3346
derivative pesticide				
Phenoxy pesticide	2765	3000	2999	2766
Phenyl urea pesticide	2767	3002	3001	2768
Phthalimide derivative	2773	3008	3007	2774
pesticide				
Pyrethroid pesticide	3349	3352	3351	3350
Thiocarbamate pesticide	2771	3006	3005	2772
Triazine pesticide	2763	2998	2997	2764

Table 2. Pesticide classes and UN Shipping Numbers

There are also generic listings for insecticide gases. Some examples are

• Insecticide gas, n.o.s., UN# 1968

- Insecticide gas, toxic, flammable, n.o.s., UN#3355
- Insecticide gas, toxic, n.o.s., UN#1967
- Insecticide gas, flammable, n.o.s., UN#1954 or UN#3354

A relatively non-toxic but flammable pesticide might be classified under UN1993.

The words "toxic" and "poisonous" are synonymous in the 2008 Emergency Response Guidebook, and n.o.s. means "not otherwise specified". However, "Liquid, toxic", "Liquid, toxic, flammable" and "Liquid, flammable, toxic" have different meanings as defined by the U.S. Department of Transportation:

- Liquid, flammable, toxic: flash point less than $23^{\circ}C [23^{\circ}C = 73.4^{\circ}F]$
- Liquid, toxic, flammable: flash point between 23°C and 61°C
- Liquid, toxic: flash point over 61°C [141.8°F]

Not all chemicals can be linked to UN ID Numbers. Some by their nature are not considered dangerous or hazardous materials, and therefore are not assigned UN ID Numbers. Others such as acetone peroxide are too dangerous to ship (shipping is forbidden by any method).

Tips on Locating Information on Chemicals Using the Internet

- Try entering the chemical name or CAS number in quotes using a computer search engine such as Google.
- Most University chemical search sites are limited to their students and facility. But the University of Akron site is open to anyone. The chemical information is in the format of an MSDS. Visit <u>http://ull.chemistry.uakron.edu/erd/</u>.
- The U.S. EPA links to finding information about particular pesticides may be found by visiting

http://www.epa.gov/pesticides/science/models_db.htm#databases.

- The government NIST Chemistry Link is <u>http://webbook.nist.gov/</u>. This does not contain MSDS or hazard information, but does contain information on names, CAS numbers, basic physical properties, and IR spectra (useful for identification by an organic chemist),
- CambridgeSoft Corporation, ChemBioFinder Data Base. The web link is <u>http://chembiofinderbeta.cambridgesoft.com/</u>. Five free trial searches are allowed after which the user must develop a user name and password, with fees charged for access to some information. Various software packages can also be purchased.
- U.S. National Library of Medicine, TOXNET (Toxicology Data Network), useful for finding detailed information on toxicity of chemicals, http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB.
- U.S. government CAMEO data base, maintained by the National Oceanic and Atmospheric Administration (NOAA), http://cameochemicals.noaa.gov/search?action=new&type=simple.

There are other websites and reference sources.

Using the PEAC tool

The PEAC tool currently contains about 130,000 different entries representing names of chemicals, synonyms, shipping names, and selected brand or trade names. Once a chemical is accessed in the PEAC tool, the PEAC user can pull up information on hazards, cleanup of spills, physical properties, personal protection information, protective action distances if the chemical becomes airborne, and reactivity information if two or more chemicals are mixed. The main screen that is displayed is a menu for locating the chemical or shipping name or UN number of interest, and a tool bar at the top for linking to other operations:

PEAC-WMD		
Eile Edit Iools <u>H</u> elp		
9.48 <u>**</u> 10 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	<u>7</u> 8	
Lookup By: Name		
Lookup:	Chemical Information	•
(((2:ETHYLHEXYL)OXY)METHYL)OXIRANE ((1,1-DIMETHYLETHOXY)METHYL)OXIRANE	Chemical	-
((2.2.2-TRICHLORO-1-HYDROXYETHYL) DIM ((2-BROMO-2)NITROETHENYL)BENZENE ((2-CHLOROPHENYL)METHYLENE)PROPAN	Information	_
((2-METHYLPHENOXY)METHYL)OXIBANE ((2-PROPENYLOXY)METHYL)OXIBANE	2-ETHYLHEXYL	
((4-(1-METHYL-1-PHENYLETHYL)PHENOXY)I ((4-BIS(P-(DIMETHYLAMINO)PHENYL)METH	GLYCIDYL	-
	ETHER	<u> </u>
(((2-ETHYLHEXYL)0XY)METHYL)0XIBANE		_

The chemical or even a partial name of the chemical can be typed in under "Lookup", or alternatively the user can pull down a screen under "Lookup By:"

PEAC-WMI				
	♦ ● ID III ■ III ● ● ●	- 1	<u><u>7</u> ⊗</u>	
Lookup By:	Name 🗾			
Lookup:	Name UN Number CAS Number	•	Chemical Information	•
((2,2,2-TRIC ((2-BROMO- ((2-CHLORC	Chemical Warfare Biological Warf		Chemical Information 2-ETHYLHEXYL GLYCIDYL	
(ACETOACI	Pesticides	-	ETHER	-
GI	Glossary			_
	ERG 2008 F CHRIS Manual F MMG Chemicals			

A drop-down menu is displayed which organizes information into categories. The user can select the chemical by name, the CAS number, UN or NA Number. If Chemical Warfare, Biological Warfare, Pesticides, Explosives, etc. a shortened laundry list is displayed on the screen from which a selection can be made, or the user can simply type in the CAS#, UN or NA#, or the name of the chemical. If "ERG 2008" is selected, the ERG 2008 reference source is displayed. If CHRIS Manual is selected, the data base in the Department of Transportation and U.S. Coast Guard, Chemical Hazard Response Information System (CHRIS) is pulled up.

The next version of the PEAC tool about to be released has a search feature where the user only need to enter a partial name which can appear anywhere within the full name, and all PEAC entries where the user-entered characters will be displayed. Earlier PEAC tool additions did not have this kind of search feature.