Technically Speaking

Those Confusing Chemical Names

by John S. Nordin, Ph.D.

Have you ever been given a name or a partial name of a chemical and tried to get information about that chemical? Maybe you have heard about some chemical spill or a terrorist threat or some chemical seized in a drug raid. You tried to locate the chemical name using the PEAC tool, or the ALOHA database, or using the NIOSH pocket guide, or some other reference. You may find some chemicals with similar sounding names but not quite the one you are looking for. Maybe you found something in a reference source but are not sure if it is the right one.

Why the Confusion?

There are perhaps close to 10 million different chemicals that have been named. In addition, many of the individual chemicals are known by different names. A manufacturer may mix several chemicals together to come up with a product. Gasoline as used by the public, for example, is a mixture of about 200 different chemicals. Even the technical grade chemicals manufactured at a chemical plant may contain impurities or may contain various additives (to prevent oxidation, polymerization, etc.). Add to this the problem of language between different countries.

If you are confused, you are not alone. Even chemists might spend hours trying to track down the name of some obscure chemical.

Let us look at an example. The chemical is (4-chloro-2-methylphenoxy)acetic acid. If you are checking a reference list where the chemicals are arranged in alphabetical order do you look under "acetic acid, (4-chloro-2-methylphenoxy)- ", should you look under "chloro" and ignore the numbers, or maybe there is a separate listing for chemicals that start with numbers. This chemical also has many different names. It is also called [(4-chloro-o-tolyl)oxy]acetic acid; (2-methyl-4-chlorophenoxy)acetic acid; 4-chloro-o-toloxy)acetic acid; 2-(4-chloro-2-methylphenoxy)acetic acid; 2-methyl-4-chlorophenoxymethylacetic acid; chloro(O-cresoxy)acetic acid; chloro-(O-tolyloxy)acetic acid; and methyl chlorophenoxy acetic acid. Can't this chemical be given a simpler name? It happens that this particular chemical is a herbicide which is given the name "MCPA" in the United States. It is also called 2,4-MCPA. Other countries may have other names such as "metaxon" in Russia. Manufacturers worldwide use MCPA in their herbicide formulations which go under such names as Agroxon, Agroxone, Anicom kombi, Anicon-M, B-Selektonon M, Chwastox, Dicopur-M, Emcepan, Hedapur M52, Hedarex M, Hedonal M, Herbicide M, Leuna M, Mephanac, Methoxone, Netazol, Okultin M, Agritox, Bordermaster, Chiptox, Cornox-M, Dikotes, Dikotex, Hornotuho, Kilsem4k-2m, Krezone, Linormone, Raphone, Rhomenc, Rhomene, Rhonox, Trasan, Weedar, and Zelan. This list is not complete.

With all the different names floating around, is there any chance of doubling up, where two different chemicals are called by the same name? Yes, unfortunately this sometimes happens especially where when acronyms are used to abbreviate names. It's easy to remember a name which has been abbreviated to only a few letters rather than a long "official" chemical name, but sometimes these shortened abbreviations get used more than once. For example the name "tritonal" is used to designate an explosive made from TNT and

powdered aluminum and cast as a solid. Tritonal is also the name of an unrelated drug (a controlled substance used as a depressant).

How Many Chemicals are Important to HazMat?

Almost all of the approximately 10 million chemicals known to exist have been produced or isolated in very small quantities and are not likely to be of any concern to public safety. Chemicals that are produced in larger quantities are of concern. There are roughly 8000 or 10000 different chemicals produced in quantities over 10,000 lbs/year. Add to this perhaps a list of maybe a hundred biotoxins and chemical warfare agents and precursors which might potentially be part of a terrorist arsenal. Add another short list which might be part of an illegal drug trade. Also add a couple of hundred toxic chemicals (such as PCBs and a few pesticides) which are no longer commercially produced in the U.S. but an old stockpile or a dumpsite might be encountered.

Chemical Abstract Service Registry Number (CAS#)

Each chemical is assigned a unique CAS# by the American Chemical Society. Not every chemical known has been assigned a CAS#, but if a scientist has done any work on the chemical and publishes his/her results a CAS# will be assigned. Researchers using the Chemical Abstracts (a publication of the American Chemical Society) use the CAS# to locate publications on that chemical. For the MCPA herbicide example given, the CAS# is 94-74-6. No other chemical has this number. The first field (e.g. 94 in the example) can have any number 50 or higher. The second field can be any number from 00 to 99. The third field is a digit from 0 to 9. The lowest possible number is 50-00-0, which is assigned to formaldehyde. Sometimes a CAS# is assigned to a mixture of chemicals and the individual components of the mixture might also be assigned their individual CAS numbers. This is done with petroleum distillation fractions (jet fuels, naphtha solvents, etc.).

When trying to identify and locate information about a chemical, half the battle is won if the CAS# can be identified. This is the one check between reference sources to make sure that we are talking about the same chemical.

Chemical Formula (Hill System)

The chemical formula gives information as to what elements (atoms) make up the chemical molecule. There are approximately 90 different elements which occur naturally plus a number that are man-made. Most people have at some time seen a Periodic Table of the Elements which display the elements arranged in groups. The elements are represented by symbols, e.g. H for hydrogen, C for carbon, S for sulfur, Cl for chlorine, Na for sodium, Fe for iron, K for potassium, etc.. Scientists worldwide use the same symbols to represent the elements even though the elements may have different names in different languages. For example, methane is made up of one atom of carbon and four atoms of hydrogen; the chemical formula is written CH_4. The chemical 2,2-dichloropropionic acid has the chemical formula (as listed in the NIOSH pocket guide to Chemical Hazards) CH_3CCl_2COOH. Another name given to this chemical is dalapon. There are a total of three atoms of carbon, four atoms of hydrogen, two atoms of chlorine, and two atoms of oxygen in the 2,2-dichloropropionic acid molecule. The formula is written this way to display how the atoms are arranged in the molecule. The formula for propionic acid is CH_3CH_2COOH. But two chlorine atoms have been substituted for two of the hydrogen atoms attached to the second carbon atom in 2,2-dichloropropionic acid.

The Hill system of representation of a chemical formula makes no distinction of how the elements are arranged within the molecule but simply counts the number of atoms of each element. By convention, carbon atoms are listed first. Second in order are hydrogen atoms. All other elements are listed in alphabetical order. For the 2,2-dichloropropionic example, the Hill representation would be $C_3H_4Cl_2O_2$. Sometimes this is written as C3H4Cl2O2 or C3H4(Cl)2O2. Another chemical, 1,2-dichloropropionic acid, $CH_2ClCHClCOOH$, would be also be represented by $C_3H_4Cl_2O_2$ in the Hill system. Chemicals which have the same chemical formula (as represented by the Hill system) but the elements are arranged differently are called isomers.

Why is the Hill system important? Many reference sources arrange their chemicals using the Hill system. The chemicals without carbon atoms are listed first, arranged in alphabetical order according to their chemical formulae. After these are listed all the chemicals with one carbon atom, then two carbon atoms, etc.. These reference sources also provide cross-references with CAS#, Hill representation of the chemical formula, and a few of the most common names. An example of a reference source which organizes chemicals according to the Hill system is

T.E. Daubert and R.P. Danner, 1992. Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. American Institute of Chemical Engineers and National Standard Reference Data System. Hemisphere Publishing Corporation.

This reference was heavily consulted for physical and thermodynamic properties when developing the PEAC tool calculations of evaporation rates of spilled chemicals.

Isomers

Isomers are chemicals which have the same chemical formula as represented by the Hill system but the atoms (elements) are arranged differently. The isomers also have different melting points, different boiling points, and may display different toxicity. They are different chemicals but have the same chemical formula. For example, let us list the isomers with the chemical formula $C_6H_{12}O$ (sometimes written as C6H12O in lists). These chemicals have six carbon atoms, 12 hydrogen atoms, and one oxygen atom arranged in various ways.

Isomers of C6H12O

Common name	CAS#	Structural Formula
Butyl vinyl ether	111-34-2	CH3CH2CH2OCH2CHCH2
Cyclohexanol	108-93-0	(CH2)5CHOH
Ethyl isopropyl ketone	565-69-5	(CH3)2CHCOCH2CH3
1-hexanal	66-25-1	CH3(CH2)4CHO
2-hexanone	591-78-6	CH3OCH2CH2CH2CH3
3-hexanone	589-38-8	CH3CH2CH2COCH2CH3
Methyl isobutyl ketone	108-10-1	CH3COCH2CH(CH3)2

The chemicals may have more then one common name. Butyl vinyl ether also goes by the names 1-(ethenyloxy)butane and N-butyl vinyl ether. 1-hexanal also is known by the names hexaldehyde, caproaldehyde, and n-hexyl aldehyde. When doing a search to find out information about a chemical, it is important to check the CAS# to make sure we are talking about the same chemical as the chemical may be listed under different names in different

reference sources.

Chemical Warfare Agents

The military sometimes uses one or two letter designations for chemical warfare agents and their precursors. The following table might help in finding information about these chemicals:

Abbreviation	CAS #	Name(s)
AC	74-90-8	Hydrogen cyanide
BZ	6581-06-2	3-Quinuclidinyl benzilate; TNB
CA	5798-79-8	Bromobenzyl chloride
CG	75-44-5	Phosgene
CK	506-77-4	Cyanogen chloride
CN	532-24-4	Chloroacetophone
CS	2698-41-1	O-Chlorobenzylidene malononitrile
CX	1794-86-1	Phosgene oxide
DA	712-48-1	Diphenylchlorarsine; Clark I
DC	23525-22-6	Diphenylcyanoarsine; Clark II
DF	676-99-3	Methylphosphonyldifluoride
DM	578-94-9	Adamsite; Phenarsazine chloride
DP	503-38-8	Diphosgene; trichloromethyl chloroformate
ED	598-14-1	Ethyldichloroarsine
GA	77-81-6	Tabun
GB	107-44-8	Sarin; isopropyl methylphosphonofluoridate
GD	96-64-0	Soman
GE		Ethyl Sarin; O-isopropyl ethylphosphonofluoridate
GF		Cyclohexyl methylphosphonofluoridate; Cyclohexyl Sarin
H	505-60-2	Mustard gas (impure); sulfur mustard (impure)
HD	505-60-2	Mustard gas (distilled); sulfur mustard (distilled)
HN-1	538-07-8	Nitrogen mustard (HN-1); ethylbis(2-chloroethyl)amine
HN-2	51-75-2	Nitrogen mustard (HN-2); N,N-bis(2-chloroethyl)methylamine
HN-3	555-77-1	Nitrogen mustard (HN-3); 2-chloro-N,N-bis(2-chloroethyl)ethanamine
HS	505-60-2	Mustard gas; bis-(2-chloroethyl) sulfide
L	541-25-3	Lewisite
MD	593-89-5	Methyldichloroarsine
PD		mixture phenyldichloroarsine and phosgene
PS	76-06-2	Chloropicrin
SA	7784-42-1	Arsine
Q	3563-36-8	Sesqui mustard; 1,2-Bis(2-chloroethylthio)ethane
QL	57856-11-8	O-ethyl O-2-diisopropylaminoethylmethylphosphonite
V-gas		An isomer of VX made in the former Soviet Union
VX	50782-69-9	O-ethyl-S-(2-diisopropyl aminoethyl) methylphosphonothiolate

Where Can You Find Information on That Chemical?

There are several Internet sources that can be checked to locate information on a chemical. If the chemical is used in industry or research a good place to start is the University of Akron (Ohio) database:

http://ull.chemistry.uakron.edu/erd/

The user enters either the CAS# or the chemical name. A listing of chemicals which closely match the user's selection is provided.

Another database is the chemfinder data base run by Cambridge Soft Corp. (Cambridge MA and Cambridge UK)

http://chemfinder.cambridgesoft.com/

Cambridge Soft. Corp. would prefer that you buy their software, but they allow a few free searches using their database.

The NTIS database is good for locating synonyms, chemical formula, and physical properties if you know the CAS #. [NTIS = National Institute of Standards and Technology, a U.S. government organization]

http://webbook.nist.gov/chemistry/cas-ser.html

If you don't know the CAS # but know the name or the Hill formula go to

http://webbook.nist.gov/chemistry

If the chemical might be used in a terrorist incident, information about such chemicals might be found at

http://www.bt.cdc.gov/Agent/agentlistchem.asp

The U.S. EPA maintains a database on chemicals registered for use as pesticides.

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

More information on chemicals used as pesticides can be found at

http://www.hclrss.demon.co.uk/index_cn_frame.html

The U.S. Food and Drug Administration maintains a search engine for doing searches on drugs:

http://www.fda.gov/search.html

If you still can't locate the information you need, try the Brookhaven National Laboratory website, and follow the instructions on the web page for access to various databases.

http://www.bnl.gov/scapa/