Lawrence H. Keith, Ph.D.
Chemistry Development Coordinator
Radian Corporation
Austin, Texas 78766

Douglas B. Walters, Ph.D.
Head, Chemical Health and Safety Section
Program Resources Branch
National Toxicology Program
National Institute of Environmental Health Sciences
Research Triangle Park, North Carolina 27709

Library of Congress Cataloging in Publication Data

Main entry under title:

Compendium of safety data sheets for research and industrial chemicals.

Bibliography: p.
Includes indexes.
1. Chemicals--Safety measures--Tables. I. Keith, Lawrence H., 1938- II. Walters, Douglas B.
TP200.C66 1985 660.2'804 84-27107
ISBN 0-89573-313-7 (set)

Printed in the United States of America.

ISBN 0-89573-313-7 VCH Publishers, Deerfield Beach (set)
ISBN 0-89573-314-5 VCH Publishers, Deerfield Beach (Part I)
ISBN 3-527-26311-X VCH Verlagsgesellschaft, Weinheim (set)
ISBN 3-527-26312-8 VCH Verlagsgesellschaft, Weinheim (Part I)

SPECIAL NOTICE
FROM THE EDITORS

The information contained herein is based upon data drawn from the literature or experimentally determined and is believed to be accurate. Great care has been taken to assure the typing, editing and accuracy of the information contained in this Compendium. However, no warranty or representation is expressed or implied by the editors or the publisher regarding the accuracy of these data or the results to be obtained from the use thereof. This applies to all of the information herein and expressly to the information in the first aid, health hazards and shipping sections.

Preface

There are many excellent compilations of chemical and physical data available as references. The same can be said of medically related reference books. Fewer references, however, are available as guides to safe usage, storage, cleanup and shipping regulations, and fewer yet that contain any information pertaining to selection of glove materials for personal protection against exposure to any but the most common of chemicals and solvents. It is the object of this **Compendium** to provide in a single source the most commonly sought and useful information for safety-oriented needs involving chemicals of both research and industry. Instead of having to search through multiple reference sources for this information, one can simply use this **Compendium.** The information herein is compiled from over fifty reference sources.

The utility of this **Compendium** has become even greater with the recent promulgation of the NIOSH Hazard Communication Rule. This ruling requires manufacturers, formulators, repackagers, distributors, and importers of hazardous chemicals or mixtures which contain as little as 1% of hazardous chemicals (and 0.1% of carcinogenic chemicals) to provide their employees with Material Safety Data Sheets (MSDSs). Most of the specific information in the MSDSs will be found in this **Compendium** for those compounds which are listed. The **Compendium** data sheets cannot be used as substitutes for MSDSs because information such as appropriate engineering controls, work practices and personal protective equipment are not included herein. However, all of the "searchable" information that is so time consuming -- and expensive -- to gather is incorporated in these **Compendium** data sheets.

The majority of the compounds in this **Compendium** are drawn from information compiled by the National Toxicology Program (NTP). The NTP was established as a U.S. Department of Health and Human Services cooperative effort to coordinate and provide information about potentially toxic chemicals to regulatory and research agencies and to strengthen the science base in toxicology. Chemicals for testing in NTP programs are screened and selected by a Chemical Selection Committee. Criteria for selection include potential for human exposure through use in manufacture, formulation and research. To these compounds the editors have added selected compounds of importance to chemical synthesis and research, The fact that most of these compounds in these volumes have also been chosen for study by the National Toxicology Program further enhances the utility of this **Compendium** by prioritizing many of the compounds that are suspected of being potentially hazardous chemicals. This does not mean that they are hazardous chemicals -- merely that they were chosen for study for one reason or another.

These three volumes contain detailed information on 867 different chemicals. It

is anticipated that supplemental volumes containing information on additional chemicals will be published in future years.

As with any reference of this kind, information and regulations are rapidly changing, particularly regarding shipping. It is therefore wise to consult the latest government regulations before using the information herein as the final reference.

Acknowledgments

The editors wish to express their appreciation to Charles E. Hudak, William S. Baillargeon, Carole Starr and Robin D. Smith for their diligent efforts in helping to prepare these data sheets and to Melody DeMoss for her patience in typing many of them. Special thanks are also extended to Virginia H. Keith who was invaluable in helping to produce the indexes and in preparing the manuscript for publication.

Contents

Part I

Part II

Part III

ABBREVIATIONS

The following abbreviations are used throughout the **Compendium.**

<	less than
>	greater than
ACGIH	American Conference of Governmental Industrial Hygienists
^{o}C	degree Centigrade
CAS	Chemical Abstracts Service
cc	cubic centimeter
chem.	chemical
CL	ceiling value for air contaminant standards
CNS	central nervous system
DEA	U. S. Drug Enforcement Administration
dec.	decomposes
DMSO	dimethyl sulfoxide
D.O.T.	U. S. Department of Transportation
Ed.	Edition
EPA	U. S. Environmental Protection Agency
^{o}F	degree Fahrenheit
F	fluorine
g	gram
gal.	gallon
Hg	mercury
Indust.	industrial
lb	pound
LCLo	lethal concentration low
LDLo	lethal dose low
LD50	lethal dose fifty (percent)
m^3	cubic meter
mg	milligram
mg/m^3	milligram per cubic meter
mL	milliliter
mm	millimeter
NIOSH	National Institute for Occupational Safety and Health
N.O.S.	not otherwise specified
OSHA	U. S. Occupational Safety and Health Administration
p	page
pp.	pages
ppm	part per million
pt.	pint
qt.	quart
STEL	short term exposure limits
temp.	temperature
TLV	threshold limit value for air contaminants
TSCA	Toxic Substance Control Act
TWA	time weighted average
ug	microgram
UV	ultraviolet light
WLN	Wiswesser Line Notation

Compendium Number

Each compound has a unique number by which it is indexed in this Compendium. This number is listed in the upper corner of each page.

NTP Preferred Name

The National Toxicology Program has a preferred name which corresponds to the name under which its computerized records are kept. This is the name under which the primary index for the compounds in this Compendium are listed; it is not always the preferred name for use by chemists. Those compounds not a part of the National Toxicology Program are listed under "Preferred Name" which is, in general, an International Union of Pure and Applied Chemistry (IUPAC) convention name.

Synonyms

Most compounds are known by more than one chemical name. The most common synonyms are listed in this section for each preferred name. The index of synonyms is a master list of all the synonyms and preferred names used in this Compendium.

CAS Registry Number

This is a unique nine digit number assigned by the American Chemical Society Chemical Abstracts Service. The CAS Number is assigned to all individual known chemical compounds and also to certain mixtures and commercial formulations.

The CAS numbers in these data sheets have been checked by a computer program. The last digit in a CAS number is the first number to the left of the decimal in the sum which is derived from (n+1) times each of the CAS numbers in sequence from right to left begining with the first CAS number to the left of the last hyphen. This is illustrated below:

CAS No. 123-72-8

1	x	2	= 2
2	x	7	= 14
3	x	3	= 9
4	x	2	= 8
5	x	1	= 5

Last Digit: 8

NIOSH Registry Number

This is an alpha-numeric nine digit number that references this compound in the 1983 (microfiche) publication, Registry of Toxic Effects of Chemical Substances, edited by R. J. Lewis. This registry is a publication of the National Institute for Occupational Health and Science (NIOSH) which lists 45,156 chemical substances.

Formula

Empirical formulas are listed wherever possible. These formulas show the number of each type of atom present in the molecules. If the compound is a salt, chelate or any other type of combination of two or more molecules in a stoichiometric ratio, including water of hydration, this is usually designated with a centered dot separating the molecules. For example, compound number 174, 4-chloro-o-toluidine hydrochloride, has the empirical formula C_7H_8ClN and HCl with the two stoichiometric entities separated by a dot instead of a combined formula represented by $C_7H_9Cl_2N$. If the formula is not able to be specifically defined because the material is a mixture of closely related molecules then either no formula is presented or a modification of the above format is used. For example, compound number 75, benzyldimethyl(mixed alkyl)ammonium chloride is designated as $C_9H_{13}N$ - RCl where RCl is an unspecified number of mixed alkyl chlorides.

Molecular Weight

The molecular weights given are formula weights, or molar masses in daltons, usually to the nearest one hundredth of an atomic mass unit (amu). These values are usually quoted from the literature if they can be found at all. They are based on multiples of the average atomic mass units listed below except for special cases involving high molecular mass substances or mixtures. Benzyldimethyl(mixed alkyl)ammonium chloride, compound 75, is such an example; its molecular weight is given as a unit range from mass 281 - 422.

Element		Mass Used	Element		Mass Used
Arsenic	As	74.922	Boron	B	10.811
Bromine	Br	79.909	Calcium	Ca	40.08
Carbon	C	12.011	Chlorine	Cl	35.453
Chromium	Cr	51.996	Cobalt	Co	58.933
Copper	Cu	63.54	Fluorine	F	18.998
Hydrogen	H	1.008	Iodine	I	126.904
Iron	Fe	55.847	Lead	Pb	207.19
Lithium	Li	6.939	Magnesium	Mg	24.312
Manganese	Mn	54.938	Mercury	Hg	200.59
Nickel	Ni	58.71	Nitrogen	N	14.007
Oxygen	O	15.999	Phosphorus	P	30.974
Potassium	K	39.102	Selenium	Se	78.96
Silicon	Si	28.086	Silver	Ag	107.870
Sodium	Na	22.999	Sulfur	S	32.064
Tin	Sn	118.69	Titanium	Ti	47.90
Uranium	U	238.03	Zinc	Zn	65.37

WLN

The Wiswesser Line Notation (WLN) is not commonly listed in other chemical reference books. Yet, with increasing use of computerized data, particularly by the pharmaceutical industry, the inclusion of WLNs becomes more important because they are alpha-numeric descriptions of the chemical structure that can be computerized easily. WLN uses numbers to express lengths of alkyl chains and the sizes of rings. These symbols then are cited in connecting order from one end of the molecule to the other. The symbols used in WLNs are the 26 capital letters, the ten numerals, the blank space and four punctuation marks (&, -, /, and *). These are all available on existing computers and card punching machines so no special equipment is needed to computerize the data. The great utility of WLNs is in computerized sorting, searching, list printing, structure-activity relationships and data retrieval.

The source used for checking all WLNs and for generating those not available was The Wiswesser Line-Formula Chemical Notation, Third Edition, by Elbert G. Smith and Peter A. Baker, (1976), Chemical Information Management, Inc., Cherry Hill, N. J., U.S.A.

Structure

Every attempt has been made to present the chemical structures of these chemicals as accurately as possible. Most chemical structures have been drawn from the American Chemical Society's Chemical Abstract Service on line structure searches, the Handbook of Chemistry and Physics or the Merck Index.

Physical Description

Whenever possible the physical description of the materials listed in these volumes was drawn from the literature. In some cases no information of this type could be found. When this situation occurred, the description used was that provided by the National Toxicology Program Chemical Repository.

Melting Point

The melting points are drawn from available literature sources and reported as a range in degrees Centigrade. Where two or more melting points are recorded the higheat or the one considered to be most probable is listed in this column. The second melting point is listed in the column Other Physical Data. Known cases of polymorphism or double melting points are noted. In a few cases melting points for cis, trans and mixtures of cis and trans isomers are provided.

Boiling Point

The boiling points are drawn from available literature sources and are reported in degrees Centigrade. If no pressure notations are included with the boiling point it is assumed that the boiling point recorded was at standard pressure (760 mm Hg). If the boiling point was obtained at a reduced pressure it is so noted directly after the temperature. When two or more boiling points at a given pressure are noted in the literature the highest temperature or the one considered most probable is listed in this column. The other boiling point is then listed in the Other Physical Data column; likewise, if data at more than one pressure is available it will also be listed in this column along with the pressure at which it was obtained.

Density

Density is the mass of a substance per unit volume. In all cases in these volumes it is the mass in grams per milliliter (cubic centimeter). Density measurements were drawn from the available literature sources or were experimentally determined.

Specific Gravity

The specific gravity of a chemical is a ratio of the mass of the chemical, solid or liquid, to the mass of an equal volume of water at a specified temperature. The usual convention is to use the mass of water at 4°C, which is the temperature at which it is at its greatest density. The first temperature listed is that at which the mass of the chemical was measured; the second temperature listed is that at which the mass of the water was measured and it is separated from the first temperature by a slash. In a few cases the specific gravity is recorded as a range. Thus, for example, the specific gravity of Acetaldehyde is listed as 0.780 to 0.790 and the masses of both Acetaldehyde and water were measured at 20°C.

Flash Point

The flash point is defined as the lowest temperature at which vapors above a volatile combustible substance will sustain combustion in air when exposed to a flame. Two methods are generally used, a Tag closed cup with ASTM Method D56 or a Cleveland open cup with ASTM Method D93. Often the method used for measurement of flash points is not indicated in literature references but when it is, C.C. refers to the closed cup method and O.C. refers to the open cup method. A general observation is that the closed cup appears to be the more commonly referenced method when it is listed. The closed cup method is also the one utilized by the NTP Chemical Repository program. Another general observation is that the open cup value is often about ten to fifteen degrees higher than the closed cup value.

Flammability

The term "flammability" in this reference is dependent on flash point. Three degrees of flammability are used: flammable, combustible and nonflammable. They are defined as follows:

Flammable - flash point is less than 100°F,

Combustible - flash point is measurable and greater than 100°F, and

Nonflammable - flash point is not measurable.

Stability

Stability refers to the propensity of the material to remain chemically unchanged during storage. Typical stability problems are sensitivities to heat, light, air and/or moisture. If a compound is unstable to any of these environmental conditions it must be handled and stored with special care to prevent degradation. If a compound is not known to be unstable to any of the above contitons it is refered to as being "stable under normal laboratory storage conditions." This means that when stored in a typical container (glass bottles for organic compounds and plastic bottles for inorganic compounds) under ambient conditions (an air conditioned or heated room about 70° - 80°F) that no appreciable chemical change or degradation (<1%) will occur over a period of several years. This definition is necessarily imprecise because of the lack of information on storage stability of most chemicals. Thus, this is a fairly subjective interpretation and is subject to change as more information is gained.

Reactivity

Reactivity is defined as chemical transformation or change that occurs when the subject material reacts with other chemicals or with itself. For the purpose of this publication it is assumed that the subject reaction occurs under essentially ambient conditions. The materials with which the subject compound will react are listed in this section. If the subject material can react with itself to polymerize, decompose or otherwise degrade, this is also noted.

Solubility

Common solvents used in toxicity testing include water, DMSO (dimethyl sulfoxide), 95% ethanol, acetone, diethyl ether and benzene. When available, solubility data is presented for each of these solvents over a specific weight per volume range using units of milligrams per liter. To be considered soluble at the referenced range all of the subject material must have dissolved in the given amount of solvent. When the solubility measurement was conducted as part of the NTP Chemical Repository program the temperature at which the measurement was made is included. If no experimentally determined solubility measurements were performed on a given compound under the NTP chemical repository program then literature references are used. The latter data is often poorly documented, highly variable, and include inconsistant definitions of terms such as "insoluble", "slightly soluble", "poorly soluble", "soluble", "very soluble" and "highly soluble".

Other Physical Data

A large variety of miscellaneous chemical and physical information is included in this section. Data involving solubilities in solvents other than the six listed in the solubility section, lower and upper explosive limits, refractive index, boiling points under reduced pressure, conflicting information on any of the above physical or chemical properties, multiple crystalline or other physical states, vapor pressure, vapor density, odor, pK, optical rotation, etc. are all listed in this section.

D.O.T. Shipping Name

The U. S. Department of Transportation (D.O.T.) has stringent rules and regulations governing the shipping and transport of chemicals. These are documented in two publications entitled "Hazardous Materials Regulations of the Department of Transportation" by the Bureau of Explosives and "Code of Federal Regulations" by the U. S. D. O. T. Specific shipping names are designated for many hazardous materials by D.O.T. These approved shipping names are required to be placed on the outside of shipping containers and in accompanying Shipper's Certification for Hazardous Wastes forms whenever chemicals are shipped in the United States or across international boundaries. The inclusion of the approved shipping name in this publication is thus of great utility for anyone who needs to transport or to ship any of the chemicals listed in these volumes for it is the responsibility of the shipper to properly and correctly assign the proper shipping name and complete all of the required shipping papers. There are over one hundred pages of tables listing specific compounds and materials classified by D.O.T. as hazardous materials for the purpose of transportation. When the subject compound is not on this list then it should be given a general descriptive approved name if possible. Examples of this situation include, "Hazardous Substance, Solid, N.O.S.", "Flammable Liquid, N.O.S.", "Poisonous Liquid, N.O.S.", etc. The abbreviation N.O.S. stands for "Not Otherwise Specified" and is a D.O.T. term. Sometimes a proper shipping name will be followed with a series of letters and numbers in parentheses. These are used to indicate the minimum quantity of that material that constitutes a reportable quantity, excluding water and other formulating materials. The units are expressed in both pounds and kilograms. For example (RQ-1000/454) means that the reportable quantity of the chemical in question is 1,000 pounds or 454 killograms.

D.O.T. Identification Number

This is a four-digit number assigned by the United Nations Committee of Experts on the Transport of Dangerous Goods to identify a substance or a particular group of substances. If a number has not yet been assigned by the UN Committee then it will consist of a D.O.T. identification number preceeded by the letters "NA". United Nations numbers are always preceeded by the letters "UN". Numbers preceeded by "UN" are associated with descriptions considered appropriate for international shipments as well as domestic shipments in the United States. Numbers preceeded by "NA" are associated with descriptions that are not recognized for international shipments except to and from Canada from the United States. If an identification number is in the "NA9000" series, it is either associated with the description of a material that is not appropriately covered by international hazardous materials shipping standards or not appropriately addressed by such standards for emergency response information purposes except for transportation between the United States and Canada.

D.O.T. Hazard Classification

Shipment or transportation of chemicals and hazardous materials also requires a correct documentation of the classification of hazard that the subject materials pose. Furthermore, if a material is defined as being subject to more than one hazard classification, the classification with the highest priority of ranking must be used. The D.O.T. hazard classifications are ranked in priority according to the following order:

1. Radioactive material
2. Poison A
3. Flammable gas
4. Non-flammable gas
5. Flammable liquid
6. Oxidizer
7. Flammable solid
8. Corrosive material (liquid)
9. Poison B
10. Corrosive material (solid)
11. Irritating material
12. Combustible liquid (in containers with >110 gallons)
13. ORM-B
14. ORM-A
15. Combustible liquid (in containers with <110 gallons)
16. ORM-E

These classifications are essentially self-descriptive except for the ORM (Other Regulated Material) and Poison classes. These are defined by D.O.T. as follows:

ORM-A is a material which has an anesthetic, irritating, noxious, toxic, or other similar property and which can cause extreme annoyance or discomfort to passengers and crew in the event of leaking during transportation.

ORM-B is a material (including a solid when wet with water) capable of causing significant damage to a transport vehicle from leakage during transportation.

ORM-E is a material that is not included in any other hazard class, but it is subject to the requirements of D.O.T. shipping regulations.

Poison A substances are gases or liquids of such a nature that a very small amount of the gas, or vapor of the liquid, mixed with air is dangerous to life; they are considered extremely dangerous poisons.

Poison B substances are liquids or solids (including pastes and semisolids), other than Class A poisons or irritating materials, which are known to be so toxic to man as to afford a hazard to health during transportation; or which, in the absence of adequate data on human toxicity, are presumed to be toxic to man because they fall within any one of the following categories when tested on laboratory animals:

* Oral Toxicity. Those which produce death within 48 hours in half or more of a group of 10 or more white laboratory rats weighing 200 - 300 grams at a single dose of 50 milligrams or less per kilogram of body weight, when administered orally.

* Toxicity on Inhalation. Those which produce death with in 48 hours in half or more of a group of rats as defined above, when inhaled continuously for a period of one hour or less at a concentration of 2 milligrams or less per liter of vapor, mist, or dust, provided such concentration is likely to be encountered by man when the chemical product is used in any reasonable foreseeable manner.

* Toxicity by Skin Absorption. Those which produce death within 48 hours in half or more of a group of 10 or more rabbits tested at a dosage of 200 milligrams or less per kilogram of body weight, when administered by continuous contact with the bare skin for 24 hours or less.

Other Shipping Regulations

These include any special notations and requirements documented in D.O.T. regulations. Common notations relate to specific labeling requirements and specific limitations on amounts of the material that can be shipped by either passenger airlines or by cargo airlines. If there are no special limits this is also documented here.

Exceptions

If there are any exceptions noted to the general regulations set forth by D.O.T. these are referenced by exact section in "Hazardous Materials Regulations of the Department of Transportation." Furthermore, the section listing specific requirements for the subject material are also included here.

Acute Hazards

Acute hazards are those that cause a specific problem within a short period of time (seconds to days). Examples are irritations to the body or toxicity that will cause sickness or death. These are distinguished from chronic hazards which cause problems over a much longer period of time (sometimes years). Examples of chronic hazards include tumors, birth defects, etc. This section is limited to acute hazards since there is much less information currently available on chronic hazards. However, in those few cases where specific chronic hazards are documented a notation to this effect is included in the section on exposure limits. When there is no information available on acute hazards for a specific compound but a reasonable estimation can be made based on its chemical class, then the acute hazard is preceeded with the word "Probably". If insufficient information is available to make a reasonable estimation of acute hazards then "Unknown" is used here. Finally, a distinction between "irritant" and "local irritant" is made in this section. A "local irritant" is defined as a material that will cause irritation upon that part of the body to which it is directly exposed. In contrast, an "irritant" is a material that will readily migrate, usually through volatilization, to other parts of the body from that part to which it was exposed. A lacrymator is thus always classed as an "irritant" while a nonvolatile solid or liquid that causes minor and localized irritation upon contact with the skin, mucous membranes, etc. is classed as a "local irritant". Due to the wide range of volatility and degrees of irritation that various materials cause these terms are by necessity somewhat subjective.

Symptoms

In general, medical terms are used in this section in an effort to be precise and to be useful to medical personnel. The disadvantage of this is that many of the terms are meaningless to the layperson with no medical training. A glossary is thus provided which defines many of these terms. If no symptoms are known then "Unknown" is used here. If no symptoms are known for the specific compound listed but symptoms are known for an isomer or a very closely related compound then the symptoms for the other compound may be used with the prefix "Probably"; reasonably accurate information is considered to be better and more helpful in a situation where aid is necessary than no information at all.