

Introduction to Chemical Data Reference Books and Calculations Part I

There are over ten million known organic compounds. Properties of several thousand of these can be found in chemical data reference books. In this experiment, you will learn:

1. Which reference books to use to find data for specific compounds.
2. Where to locate the appropriate data in the various reference books.
3. What the symbols and abbreviations found in reference books mean.
4. How to locate information on material safety data sheets (MSDS).
5. How to use the information to perform simple calculations of molar quantities, limiting reactants and yields.

A student who has prepared for this exercise should be able to:

1. The student will determine the nature and extent of information needed.
2. The student will access the needed information effectively and efficiently.
3. The student will evaluate information and its sources critically.
4. The student will demonstrate his/her information competency through writing or other modes of communication.



Background

Understanding how to use chemical handbooks and reference books is pivotal to a student's success in organic chemistry. Whether finding the melting point of a product or obtaining safety information about a reagent used in the laboratory, it will be necessary to use these reference books throughout the course. Learning to use these books efficiently will decrease the amount of time spent preparing for laboratory work. The most common chemistry reference books are the *Chemical Rubber Company Handbook of Chemistry and Physics* (CRC Press, Inc.) and the *Merck Index* (Merck & Co., Inc.), but other books, such as *Lange's Handbook of Chemistry* (McGraw-Hill), *Handbook of Tables for Organic Compound Identification* (CRC Press, Inc.), and chemical supply catalogs, such as those of Aldrich Chemical Company, Lancaster Synthesis Inc., and Fluka Chemical Company, can be used depending upon the information desired.

Handbook of Chemistry and Physics (CRC)

The CRC has much information about all fields of chemistry and physics, such as thermodynamic properties of elements, dissociation constants of acids and bases, and ionization potentials. Topics are listed alphabetically in the index in the back of the book. Of most interest to organic students is the section "Physical Constants of Organic Compounds." Physical properties such as molecular weight, boiling point, melting point, density, refractive index, and solubilities are tabulated for selected organic compounds.

Other physical data such as crystalline form, color, and specific rotation may also be included.

The data can best be understood by reading "Explanation of Table of Physical Constants of Organic Compounds" and "Symbols and Abbreviations," which can be found in the pages immediately preceding the tables. For example, the entry for acetaldehyde gives the refractive index (n_D) as 1.4409_D^{20} and the solubility as w, al. From the Explanation of Table Physical Constants of Organic Compounds, it can be seen that the refractive index is reported for the D line of sodium and that the "20" refers to the temperature at which the refractive index was measured. From the list of abbreviations and symbols, it can be seen that the compound is soluble in water and ethyl alcohol. Before starting the assignment that follows, refer to the section "physical constants of organic compounds," find these pages, and see what other information is available on organic compounds.

To find the physical properties of a given organic compound in the CRC, it is important to have a correct name. Organic compounds are listed alphabetically by their International Union of Pure and Applied Chemistry (IUPAC) names under the name of the parent compound.

The ease of use of the CRC is governed by being able to locate the parent name correctly and then to locate the substituent(s) under the parent. A comprehensive guide to naming compounds by the IUPAC system is given before the section on physical constants of organic compounds. Alternately, the compound can be located from its molecular formula in the Formula Index for Organic Compounds. However, since there are generally many organic compounds with the same molecular formula, this tends to be a tedious way to locate a compound. For example, the molecular formula of 2-methyl-1-propanol is $C_4H_{10}O$. The 63rd edition of the CRC lists reference numbers to twelve different compounds with this same molecular formula.

Merck Index

Another reference book frequently used in the organic lab is the *Merck Index*, which is an alphabetical compilation of common names of compounds, much like a dictionary. The major focus of the *Merck Index* is on pharmaceutical, medicinal, and natural products, although some common organic compounds are also included. In addition to physical properties such as molecular weight, boiling point, melting point, refractive index, density, color, crystalline structure, solubility data, and recrystallization solvents, the *Merck Index* also gives the IUPAC name, Chemical Abstracts name and alternative names, Chemical Abstracts reference numbers, toxicity and biological hazard information, biological and pharmacological information, and one or more references to the synthesis of the compound. An introductory section at the beginning of the *Merck Index* shows a sample abstract and gives abbreviations and selected definitions of the terms used in the abstract. Refer to these pages to interpret the physical data given in the abstract.

To look up a compound in the *Merck Index*, go to the index at the back of the book and find the name of the compound alphabetically. The index cross references the various names of a compound, so this is the quickest way to find the given compound. For example, the compound with the structural formula $(CH_3)_2CHCH_2OH$ is cross referenced under 2-methyl-1-propanol (the IUPAC name) and under isobutyl alcohol (a common

name). Beside each entry is an abstract number. The abstracts are numbered and arranged sequentially. Refer to the specific abstract to find information on the given compound. The *Merck Index* entry for this compound is shown here.

5146. Isobutyl Alcohol. *2-Methyl-1-propano/*; isopropylcarbinol; 1-hydroxymethylpropane; fermentation butyl alcohol. $C_4H_{10}O$; mol wt 74.12. C 64.82%, H 13.60%, O 21.58%. $(CH_3)_2CHCH_2OH$. Present in fusel oil; also produced by fermentation of carbohydrates: Baraud, Genevois, *Compt. Rend.* 247,2479 (1958); Sukhodol, Chatskii, *Spir. Prom.* 28, 35 (1962), C.A. 57, 5124e (1962). Prepn: Wender *et. al.*, *J. Am. Chem Soc.* 71,4160 (1949); Schreyer, U.S. pat. 2,564,130 (1951 to du Pont); Pistor, U.S. pat. 2,753,366; Harrer, Ruhl, Ger. pat. 1,011,865; Himmler, Schiller, U.S. pat. 2,787,628 (1956, 1957, 1957 all to BASF). Toxicity study: Smyth *et al.*, *Arch. Ind. Hyg. Occup. Med.* 10,61 (1954).

Colorless, refractive liq; flammable; odor like that of amylalcohol, but weaker. d^{15}_4 0.806. bp 108° . mp -108° . Flash pt, closed cup: $82^\circ F$ ($28^\circ C$). 1.4409^{15}_D 1.3976. Sol in about 20 parts water; misc with alcohol, ether. LD₅₀ orally in rats: 2.46 g/kg (Smyth).

Caution: Potential symptoms of overexposure are irritation of eyes and throat; headache, drowsiness; skin irritation, skin cracking. *See NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 90-117, 1990) p 132. *Use:* Manuf esters for fruit flavoring essences; solvent in paint, varnish removers.

SOURCE: *The Merck Index*, 12th ed., 1996.

Online Databases (GALILEO)

A third source of chemical information comes from online databases located on GALILEO. GALILEO is a doorway to a wealth of information. Through it you can potentially access over 150 databases indexing thousands of periodicals and scholarly journals. Over 7000 journal titles are provided in full-text. Other resources include an encyclopedia, business directories, a collection of over 10,000 full-text books and government publications. GALILEO is accessed through the Georgia Highlands Library site at <http://www.highlands.edu/academics/library/index.htm>.

One of the more useful databases for chemical information is the National Library of Medicine (NLM) and is found under the database tab. After accessing the NLM Database, you can search multiple resources for information about a specific chemical. After you have searched for a particular chemical, you will need to go to the Hazardous Substance Data Bank and select the correct chemical. And finally, under the "Chemical/Physical Properties" tab, you will find specific reference data.

Chemical Catalogs

Another source of chemical information comes from the catalogs of chemical suppliers. Although the information in these catalogs is limited, physical properties for a number of common organic, inorganic, and biochemical compounds sold by the companies are given, and the catalogs are usually easy to use. In addition to molecular weight, melting point, boiling point, refractive index, density, and specific rotation, other information such as safety hazards, disposal information, purity, and cost are also included. The physical properties are for the chemicals as supplied by the company and maybe slightly different from those for the pure compounds.

Compounds are listed alphabetically under common or IUPAC names. Thus $(\text{CH}_3)_2\text{CHCH}_2\text{OH}$ is found under 2-methyl-1-propanol in the Aldrich catalog (www.sigmaaldrich.com/).

Chemical Online Sources

Several good sources exist online. Although the information in these sources is limited, the information is very useful. The best options are:

- Flinn Scientific, Inc. at http://www.flinnsci.com/search_MSDS.asp
- ChemExper at www.chemexper.com
- PubChem at pubchem.ncbi.nlm.nih.gov

Other Sources

Other reference books such as *Lange's Handbook of Chemistry* and *The Chemist's Companion* can also be used to find specific information. In addition, there are also reference books in which spectral information about organic compounds is tabulated and others in which melting points of derivatives can be found. Your lab instructor may indicate the use of other reference books, depending upon the information desired.

The material safety data sheet (MSDS) is a good source of information about safety and other hazardous materials information. Required by law for every chemical, the MSDS provides important information about toxicity, permissible levels of exposure, health consequences of exposure, protocols for safe use, and disposal. One particularly important section of an MSDS is the Health Hazard Data section. This delivers critical information about how the chemical enters the body, the routes of entry (such as inhalation, ingestion, and skin contact), and the appropriate personal protective equipment (PPE) required to prevent exposure (such as gloves, respirator, etc.). A MSDS also lists the permissible exposure limit (PEL), which refers to the amount of exposure to a chemical that is considered safe. PELs are given as a time weighted average exposure over eight hours. The lower the PEL, the more hazardous the chemical. For example, hydrochloric acid has a PEL of 5, while ethyl acetate has a PEL of 400.

Be sure to cite all reference sources properly on all laboratory reports. The only exceptions are information in your Laboratory Manual and textbook.

Name: _____

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(Don't forget to properly cite all references. You should use a bibliography at the end of the report to do this.)

Physical Properties

When you look up physical properties, you will find a variety of abbreviations used. Explanations of symbols and abbreviations can be found in the front of the Merck Index and at the front of the Physical Properties of Organic Compounds section in the CRC. Use the Merck, CRC, or GALILEO to figure out what the following abbreviations mean.

den or d		i	
mp		alc	
n_D		cor	
dec		sl	
EtOH		aq	
misc		eth	

The boiling point of an organic compound is given in the Merck as bp₇₀ 48° and in the CRC as 48⁷⁰. What does the "70" signify? _____.

Use the **CRC Handbook** to find the following information.

n_D of pentane		density of acetic acid	
mp of benzoic acid		bp of hexane	
IUPAC name for vanillin (use CRC synonym index)			

Use **GALILEO** to find the following information (formula = molecular formula)

formula for acetone		formula for ibuprofen	
formula for benzocaine		# of double bonds in caffeine	
mp for benzocaine		mp of procaine	
density of acetone		molecular weight of propane	
formula of 2-pentanone		density of bromine	

3. Which is the limiting reagent, propane or bromine? Show your calculations.
4. Calculate the theoretical yield, in grams, of 2,2-dibromopropane.
5. Suppose that 13.88 grams of 2,2-dibromopropane were actually formed in the reaction. Calculate the percent yield of 2,2-dibromopropane.
6. Discuss the results of your search in terms of what kinds of sources you used and the likely quality of those sources. (This should be about 250 words.)