

Searching the Chemical Literature (#1a)

Introduction

The object of this laboratory is to introduce you to the various methods of locating information in the literature concerning the properties of organic and inorganic compounds. The knowledge and skills that you will acquire from this session will help you to locate the information that is needed to complete the Table of Reagents and Products in your PRELAB REPORTS. You will be introduced to a few important sources of information about organic compounds and their reactions and uses. Much of this information can be found online at the Centennial Library's website, <http://libguides.unm.edu/chem303>. Useful sources include:

1. Aldrich Catalog

Aldrich is a company that sells a wide range of organic chemicals. In the "Aldrich Catalog" all compounds are listed alphabetically and much physical and safety information is provided for each compound. Cross references (different names for the same compound, such as dichloromethane and methylene chloride) are provided in the alphabetic sequence, and there are molecular formula and Chemical Abstracts Registry Number indexes. The catalog can be accessed via the internet by going to www.sigma-aldrich.com/Brands/Aldrich.html. Use the "Product Name or No." search box to find your compound. Type the name of the compound in the search box and click "Go."

Example 1: Find the formula weight and hazardous properties of N-methylaniline.
Answer: Look up N-methylaniline and find the formula weight is 107.15 g/mole. Furthermore, it is toxic to very toxic and hazardous to the environment.

When looking up chemicals, ignore letters and numbers that indicate position (for example: N-, 2,3-, cis-) until you need to differentiate between isomers, so for N-methylaniline, look under "M," not "N."

Note that hazard information is given as a graphic icon and a series of risk and safety statements. These symbols and codes are explained beginning on page 6 of the print catalog or by clicking on the symbol in the online catalog. For our purposes, the general hazard is sufficient, but if you were going to be using the compound in the lab, it would be a good idea to review the appropriate risk and safety statements.

Example 2: What are the melting point, boiling point, and density of isobutyric anhydride and 3-isochromanone?

Answer: Look up isobutyric anhydride and find that the melting point (mp) is -56°C , boiling point (bp) is 182°C , and density is 0.954 g/mL at 25°C . Look up 3-isochromanone and find that the melting point is $80\text{-}82^{\circ}\text{C}$. The boiling point and density are not given.

Note that the Aldrich Catalog *generally* does not give densities and sometimes does not give boiling points for solids. The melting point of 3-isochromanone is above room temperature (20-25°C), so the compound is a solid at room temperature.

2. CRC Handbook of Chemistry and Physics

In addition to many other tables of chemical and physical properties, the "CRC Handbook of Chemistry and Physics" (or just "CRC") tabulates physical properties and other data for many common organic compounds. This table is Section 3 of the handbook. All abbreviations (except that you're expected to know H₂O) used in this table are explained in a list at the beginning of the table, on page 3-2. If your compound is not listed under the name you are given, try the Synonym Index at the end of the table. (The page number for the synonym index changes each year.) The CRC also has Molecular Formula and CAS Registry Number Indexes to the Physical Constants of Organic Compounds table.

Example 3: Find the melting and boiling points of 2-*tert*-butyl-5-methylphenol.

Answer: Look up the compound (under "b" for butyl, not "t" for *tert*) and look across to find the melting point given as 46.5°C and a boiling point of 127°C. The superscript of "11" on the boiling point is the pressure in mm Hg at which the measurement was obtained and should be included when you give the boiling point.

Example 4: Find the solubility of 2-nitronaphthalene.

Answer: Look up the compound and read across to the last column. The solubility is given as "i H₂O; vs EtOH, eth," which translates to "insoluble in water; very soluble in ethanol and diethyl ether."

Example 5: Find the density of caprolactone.

Answer: "Caprolactone" is not listed in the alphabetic list, so check the synonym index. It is listed in the synonym index a referred to "8443" (in the 2003-2004 edition). Going to *line number* 8443 in the table, you will find a listing for 2-oxephanone and caprolactone listed in the second (synonym) column. Reading across, the density is given as 1.0761 g/cm³. The superscript "20" indicates that the density was measured at 20°C.

Please note that the format of the Physical Constants of Organic Compounds table changed dramatically with the 84th edition (2003-04). If you use an older version, the table is still section 3, but compounds are listed under a "parent-comma-derivative" format, so you would look for "2-chloromethylbutane" under "b" for "butane, 2-chloromethyl-," and "2-chloromethylbutane" would likely be listed in the synonym index. Data for each compound are also given in a two-line format in the older versions.

3. Materials Safety Data Sheets

Material Safety Data Sheets (MSDSs) contain detailed and useful safety information on chemicals. MSDS information can be found on a CD in the Centennial Library, and many can be found by googling "msds" and the name of the compound. When using MSDSs from the internet, many may be highly abbreviated and lack important information, so be sure to select

one with a reasonable amount of detail. Note that the library's CD does **not** give hazard numbers; if using the CD, summarize the major hazards associated with the compound.

The official MSDS form is divided into several sections, among them: Section 1 provides product identification, which includes various names by which the compound is known, the formula of the compound, and the CAS Registry Number. Section 3 provides a summary of hazard information, ratings with regard to toxicity, flammability, reactivity and physical contact, and detailed information on specific risks. The number 0 is a low hazard rating, whereas 4 is a severe hazard rating. Section 4 provides first aid information in case of contact with the compound. Section 6 provides information on clean-up of spills. Sections 7 and 8 provide information on storage and handling of the compound, including recommended personal protection equipment. Section 9 provides basic physical property information. Section 10 provides stability and reactivity information. Section 12 provides information on environmental hazards and fate. Section 13 provides disposal considerations for the compound or container.

Example 6: What are the hazards associated with aluminum chloride and how should it be handled?

Answer: By googling "msds aluminum chloride," locate an MSDS form for this compound. This chemical has health, reactivity, and contact hazard classifications of 1 (slight) and a flammability rating of 0 (none). The actual hazard numbers are not given on the library's CD. It may "emit toxic chloride fumes when heated to decomposition." When handling this compound wear goggles, gloves, and a lab coat and use it in a hood.

“Postlab” Assignment 1a for Searching the Chemical Literature

You will be given a slip of paper with 5 numbered compounds. The numbers correspond to the questions, which also correspond to a specific source of information. Use the compounds on your slip to answer questions 1-3. In each question, “Compound” is simply the name on your slip. If any information requested in this exercise is not given in the source used, you may write “N/A.”

You should write all of this information **in your lab notebook for your “postlab” report**. The format for this report is slightly different from the regular postlab reports for experiments. You must attach the slip of paper with your assigned compounds to your postlab report. **Failure to do so will result in a 5 point deduction from your total score.** Your report should have:

Title: Write your name, title of the assignment, section number and date on each page (1 pt)

Purpose/objective: Write a brief statement on the objective of this assignment (2 pts)

Methods: Write a description of the methods you will use to complete this assignment (2 pts)

Postlab Questions

1. Using the Aldrich Catalog, make a table with the properties for the two compounds assigned to you (14 pts). The headings for the table are shown below.

Compound	CAS #	MW, (g/mol)	Mp, (°C)	Bp, (°C)	Density, (g/mL)	Hazards	Liquid/solid
1.							
2.							

2. Using the CRC Handbook make a table for the two compounds assigned to you (14 pts). The headings for the table are shown below. Note that the codes for solubility can indicate that the compound is anywhere from slightly soluble to insoluble in the solvent. You should give solubility in words, not the codes, using the key at the front of the section (physical constants of organic compounds).

Compound	CAS #	MW, (g/mol)	Mp, (°C)	Bp, (°C)	Density, (g/mL)	Solubility	Liquid/solid
1.							
2.							

3. Using an MSDS (Material Safety Data Sheet) locate the following information about the compound listed on your assignment sheet (6 pts):

- Hazard ratings and what their values mean
- Disposal and handling precautions associated with the compound
- what you should do if this compound contacts your skin or if there is a spill of the compound in the lab