Searching the Chemical Literature (Assignment #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. Sigma-Aldrich

Sigma-Aldrich is a company that sells a wide range of organic chemicals. In the printed “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 online catalog can be accessed via the internet by going to http://www.sigmaaldrich.com/chemistry.html. Type the name of the compound in the search box at the top of the page to find your compound.

**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 Safety & Documentation, then each icon 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 80-82°C. The boiling point and density are not given.
Note that Sigma-Aldrich 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 printed 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.

Although there is a limit of two concurrent users, UNM also maintains access to the online version of the CRC Handbook. This can be found by first going to the Centennial Science and Engineering Library home page: http://library.unm.edu/about/libraries/csel.php. Click on Databases, then scroll to CRC Handbook of Chemistry and Physics. Click on the link and you will be taken to the CRC online handbook if there is an available slot. On the left tab that appears, under Table of Contents, click on the + next to Section 3, Physical Constants of Organic Compounds, then Interactive Table. You can narrow down the field by clicking on the funnel symbol to filter data by name or other property, then clicking Apply Filter after you have entered information. Note that you can position the cursor with the mouse to hover above each of the categories and see the definitions of the abbreviations.

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 type in “caprolactone” for Synonym under the filter menu. 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.
3. Safety Data Sheets

Safety Data Sheets (SDSs) contain detailed and useful safety information on chemicals. All can be found by googling “sds” and the name of the compound. When using SDSs from the internet, many may be highly abbreviated and lack important information, so be sure to select one with enough detail to help you solve the problem you want to solve. Sigma-Aldrich will be a good source of these but they are sometimes not a very good source of information about physical properties. They are often consulted when a chemical spill or fire has occurred. Usually the first question asked by hazardous materials officials or firefighters is, “Where are your SDS?” because they want to know what might have spilled or ignited.

The official SDS 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 2 provides a summary of hazard information using the Global Harmonization System. In this system hazard and precautionary statements provide guidance on how to best work with the compound. Often pictograms are used to describe the various hazards and precautions:

![GHS Pictograms & Hazards](image)

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. Sections 11 and 12 provide 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 “sds aluminum chloride,” locate an SDS form for this compound. In addition to the health hazard and corrosion pictograms, you read:

*Causes severe skin burns and eye damage. Causes serious eye damage. Causes damage to organs (Lungs) through prolonged or repeated exposure if inhaled. May cause damage to organs (Central nervous system) through prolonged or repeated exposure if swallowed. Harmful to aquatic life.*

*Do not breathe dust/ fume/ gas/ mist/ vapours/ spray. Wear protective gloves/ protective clothing/ eye protection/ face protection. Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.*

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 should have 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 Sigma-Aldrich online or the printed 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.

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS #</th>
<th>MW, (g/mol)</th>
<th>Mp, (°C)</th>
<th>Bp, (°C)</th>
<th>Density, (g/mL)</th>
<th>Hazards</th>
<th>Liquid/solid</th>
</tr>
</thead>
</table>
2. Using the printed CRC Handbook or the online CRC, 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).

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS #</th>
<th>MW, (g/mol)</th>
<th>Mp, (°C)</th>
<th>Bp, (°C)</th>
<th>Density, (g/mL)</th>
<th>Solubility</th>
<th>Liquid/solid</th>
</tr>
</thead>
<tbody>
<tr>
<td>2A.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2B.</td>
<td></td>
<td></td>
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<td></td>
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</tr>
</tbody>
</table>

3. Using an SDS (Safety Data Sheet) locate the following information about the compound #3 listed on your assignment sheet (6 pts):
   a) The hazards of this compound in words, not codes
   b) Disposal and handling precautions associated with the compound
   c) What you should do if this compound contacts your skin or if there is a spill of the compound in the lab