

# CHEMISTRY RESOURCES

Chemists frequently need to perform literature searches to find physical, chemical and spectroscopic properties of substances. Properties are needed to help identify substances and to select substances for specific applications. The literature is also a source for organic synthesis instructions. When attempting to perform a chemical synthesis, it would be senseless to ignore all of the research that has been reported in the literature. A quality literature search will enable you to learn from the experiences of others and arrive at the optimal conditions for a reaction in a much shorter amount of time. As Isaac Newton said, "If I have seen farther than others, it is because I have stood on the shoulders of giants." A good working knowledge of the literature puts you on the shoulders of the chemists who have preceded you. The importance of knowing how to access the huge and ever growing amount of chemistry literature cannot be understated.

Literature references can generally be divided into two categories, primary sources and secondary sources. The primary literature references are most commonly the journals that contain the direct reports of the research scientists such as the *Journal of the American Chemical Society*. Searches of information from primary journals usually involves use of an abstracting service such as *Chemical Abstracts*. *Chemical Abstracts* is generally available in university libraries but is very expensive and not usually available in community college libraries. Online access to *Chemical Abstracts* is also expensive. In this course, most of your literature searches will be in secondary sources such as the *Handbook of Chemistry and Physics* or the *Aldrich Chemical Catalog* and many valuable sites on the Internet. Secondary sources compile data from primary sources into condensed formats and handier tables. In some cases, especially for Internet sites, it is possible that the reference should be considered a tertiary source as the data has been collected from secondary sources. In any event and most importantly, whenever you are writing research articles, most citations should be to primary sources as there are occasional errors made whenever data is compiled.

**Compilations of Properties.** In almost all of the experiments you will perform in this course, you will need to look up intensive (do not depend on the amount of the substance) physical property data (e.g., density, melting point, boiling point, refractive index) to help you identify substances. College libraries usually will have some of the secondary references listed below. Note that most chemistry books are catalogued in the QD section (or 500 in the Dewey decimal system) of the library although a few are in the physics QC section. It is worth your time to browse the QD part of your library's reference section to give you an idea of which references are available. For each of these references, you will have to learn the fastest way to find data. It is sometimes difficult to figure out what to look for in the index for the *Handbook of Chemistry and Physics*. For properties of organic compounds, just open up the book to about the 1/3 point and you will find yourself in the middle of a huge section entitled "Physical Constants of Organic Compounds." The problem now is determining how the compound has been named by the compiler. The *Handbook* uses a system that might make it difficult for you. An alternative is to use the *Aldrich Chemical Catalog*. This commercial catalog includes the physical properties of the organic compounds sold by the company and the Aldrich nomenclature system is similar to the system you will learn in this course. Ask your instructor if there is an *Aldrich Chemical Catalog* available to put in your laboratory. The references listed below are among the best sources of secondary data.

*Handbook of Chemistry and Physics*, CRC Press, Boca Raton.

*Handbook of Chemistry*, McGraw-Hill, New York.

*Dictionary of Organic Compounds*, Chapman and Hall, London.

*Merck Index*, Merck, N.J.

*Aldrich Chemical Catalog*, Aldrich, Milwaukee.

While you probably do not own one of the above references, chances are that you have access to a computer with online access. The Internet has many sites that contain physical properties of substances. Some present the data directly when you input the name of the compound. In addition, many sites contain hotlinks to MSDS (Material Safety Data Sheet). The MSDS usually contains property data in the 9<sup>th</sup> section on physical properties. MSDS also contain toxicity information that will be needed to complete *Exercise 3*. Probably the most complete and versatile of the sites is the Knovel Critical Tables. It will be well worth your time to register at the site and familiarize yourself with the contents. Hot links to most of the sites are available at the *Organic Chemistry Directory*.

**Organic Chemistry Directory** - <http://murov.info/orgchem.htm>

### 1. Tabulation + MSDS

Acros - [http://www.acros.com/portal/alias\\_\\_Rainbow/lang\\_\\_en/tabID\\_\\_21/DesktopDefault.aspx](http://www.acros.com/portal/alias__Rainbow/lang__en/tabID__21/DesktopDefault.aspx)

Aldrich, Sigma - <http://www.sigmaaldrich.com/>

Alpha Chemical - [http://www.alfa.com/alf/laboratory\\_chemical\\_suppliers.htm](http://www.alfa.com/alf/laboratory_chemical_suppliers.htm)

ChemicalBook - <http://www.chemicalbook.com/>

ChemExper Chem. Directory - <http://www.chemexper.com/>

Chemidplus - <http://chem.sis.nlm.nih.gov/chemidplus/>

or <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

Chemspider - <http://www.chemspider.com/>

EMD Chemicals - [http://www.emdchemicals.com/corporate/emd\\_corporate.asp](http://www.emdchemicals.com/corporate/emd_corporate.asp)

Fisher - <https://new.fishersci.com/wps/portal/HOME>

TCI America - <http://www.tciamerica.com/brochure/catalog.html>

Wikipedia - [http://en.wikipedia.org/wiki/List\\_of\\_organic\\_compounds](http://en.wikipedia.org/wiki/List_of_organic_compounds)

[http://en.wikipedia.org/wiki/List\\_of\\_inorganic\\_compounds](http://en.wikipedia.org/wiki/List_of_inorganic_compounds)

### 2. MSDS

JT Baker & Mallinckrodt (primarily inorganic chemicals) -

<http://www.mallbaker.com/Americas/catalog/default.asp>

MSDSprovider - <http://www.msdsprovider.com/>

MSDS Solutions - <http://www.msds.com/>

Vermont Safety Information Resources, Inc. - <http://hazard.com/msds/>

### 3. Tabulation

Chemblink - <http://www.chemblink.com/>

Chemfate - <http://www.syrres.com/esc/chemfate.htm>

Chemical Database - <http://ull.chemistry.uakron.edu/erd/>

Chemland 21 - <http://www.chemicalland21.com/listaz01.htm>

CIS - <http://www.ilo.org/legacy/english/protection/safework/cis/products/icsc/dtasht/index.htm>

Datalog - <http://www.syrres.com/esc/datalog.htm>

Knovel Critical Tables (free registration required) -

[http://www.knovel.com/web/portal/browse/display?\\_EXT\\_KNOVEL\\_DISPLAY\\_bookid=761](http://www.knovel.com/web/portal/browse/display?_EXT_KNOVEL_DISPLAY_bookid=761)

Select the Table for *Basic Physical Properties of Chemical Compounds* and register.

Use the sort by ascending or descending order capability for any parameter and also the filter capability.

LookChem - <http://www.lookchem.com/>

National Physical Laboratory - [http://www.kayelaby.npl.co.uk/chemistry/3\\_3/3\\_3.html](http://www.kayelaby.npl.co.uk/chemistry/3_3/3_3.html)

PubChem - <https://pubchem.ncbi.nlm.nih.gov/>

Toxnet - HSDB - <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>

all Toxnet databases - <http://toxnet.nlm.nih.gov/>

WolframAlpha - <http://www.wolframalpha.com/>

**Spectroscopic Collections.** During this course, you will frequently be determining the ir, nmr and sometimes the uv-vis spectra of compounds. These spectra will be of immense help in many ways in the laboratory. First, the spectra are useful for verifying the identity of a substance. Second, for unknowns, the spectra will enable you to determine which, if any, functional groups are present in the molecule and provide considerable structural information. To verify the identity of a substance, you will need to compare an experimental copy of a spectrum to one published in the literature. There are huge catalogs of published spectra including the voluminous Sadtler Index and the more reasonably sized Aldrich libraries of ir and nmr spectra. For the latter, you can tell if the Aldrich collection contains the spectrum by looking up the compound in the Aldrich Chemical catalog. Check the QD part of the reference section of your library to see if these spectra collections are present in your library.

Fortunately, the Internet also contains several good collections of spectra. Spectra of most of the compounds you will use in this course can usually be found in at least one of the Internet collections. Particularly valuable with ir, nmr and mass spectra of many compounds is the *National Institute of Advanced Industrial Science and Technology* (referred to henceforth as NIMC) site. This is generally the first place to look. The only minor problem with the site is that it does not recognize all the possible names of a compound (you will find that organic compounds usually can be named in more than one way). If the compound is not found by name, then enter its formula. The next screen will contain a list of all the compounds with the entered formula and you will have to figure out if one of them is the compound you are looking for. Links to these sites are available at the ***Organic Chemistry Directory***.

#### Spectra (Collections)

##### 1. IR - Liquid or Solution

NIMC site - [http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre\\_index.cgi](http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi)

NIST site - <http://webbook.nist.gov/chemistry/>

RSC - <https://www.le.ac.uk/spectraschool/>

PSLC - <http://pslc.uwsp.edu/>

Chinese site - <http://www.basechem.org/>

fee based - <https://ftirsearch.com/default3.htm>

##### 2. IR - Gas Phase - NIST - <http://webbook.nist.gov/chemistry/>

##### 3. IR - Predicted - <http://www.knowitall.com/academic/welcome.asp>

##### 4. HNMR - Experimental

NIMC site - [http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre\\_index.cgi](http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi)

RSC site - <http://www.le.ac.uk/spectraschool/>

PSLC - <http://pslc.uwsp.edu/>

Chinese site - <http://www.basechem.org/>

Solvents - <http://www.alsnotebook.com/chlorformtraces.html>

##### 5. HNMR - Calculated - ChemExper Chem Directory - <http://www.chemexper.com/>

##### 6. <sup>13</sup>CNMR - Experimental

NIMC site - [http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre\\_index.cgi](http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi)

RSC - <https://www.le.ac.uk/spectraschool/>

## 7. Mass

NIMC site - [http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre\\_index.cgi?lang=eng](http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng)

NIST site - <http://webbook.nist.gov/chemistry/>

Pherobase - <http://www.pherobase.com/database/compound/compounds-index.php>

RSC - <https://www.le.ac.uk/spectraschool/>

PSLC - <http://pslc.uwsp.edu/>

Chinese site - <http://www.basechem.org/>

## 8. UV-Vis

NIST site - <http://webbook.nist.gov/chemistry/>

OMLC - <http://omlc.ogi.edu/spectra/PhotochemCAD/html/alpha.html>

RSC - <http://www.le.ac.uk/spectraschool/>

9. Bibliography - <http://library.buffalo.edu/libraries/asl/guides/spectra.html>

**Unknowns.** Several times in this course, you will probably be given unknowns and asked to identify them. Ways of approaching this problem are discussed later but the following sites enable you to input some of the physical and spectroscopic properties you have determined. The site will then scan its library and give you a list of possible hits. Be careful using these sites as they have limited libraries and may not contain your unknown. Additionally, if you enter data for a compound that is in the library but hasn't had that particular property entered, the site may not list the compound as a possibility.

Acros - [http://www.acros.com/portal/alias\\_\\_Rainbow/lang\\_\\_en/tabID\\_\\_36/DesktopDefault.aspx](http://www.acros.com/portal/alias__Rainbow/lang__en/tabID__36/DesktopDefault.aspx) (formula, structure, molecular mass, bp, mp, refractive index, density, ir)

Aldrich - <http://www.sigmaaldrich.com/catalog/search/SubstructureSearchPage> (formula, structure, molecular mass, mp, bp, density)

ChemExper Chem Directory - <http://www.chemexper.com/> (under "power search" formula, structure, molecular mass, bp, mp, refractive index, density, ir, nmr)

Chemspider - <http://www.chemspider.com/PropertiesSearch.aspx> (formula, molecular mass)

ChemIDplus - <http://chem.sis.nlm.nih.gov/chemidplus/> (formula, mp, bp)

Knovel Critical Tables (free registration required). This site will not search for a compound but because of the ability to sort properties by ascending or descending order coupled with the use of the filter capability, this site can be used to narrow down possible unknowns very quickly.

[http://www.knovel.com/web/portal/browse/display?\\_EXT\\_KNOVEL\\_DISPLAY\\_bookid=761](http://www.knovel.com/web/portal/browse/display?_EXT_KNOVEL_DISPLAY_bookid=761)

Select the Table for *Basic Physical Properties of Chemical Compounds* and register.

NIMC site - [http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre\\_index.cgi](http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi) (formula, molecular mass, ir, nmr, ms)

Organic Chemistry Data Base - <http://www.colby.edu/chemistry/cmp/cmp.html> (formula, molecular mass, mp, bp, density, refractive index, ir, ms)

**Synthesis.** There are many primary and secondary sources of synthetic procedures available. Some of the most common secondary sources are listed below.

*Organic Synthesis*, Wiley, New York, 1941 - present.

*Organic Reactions*, Wiley, New York, 1942 - present.

Vogel, A. I., et. al., *A Textbook of Practical Organic Chemistry*, 5<sup>th</sup> ed., Prentice Hall, 1989.

Fieser, L. F.; Fieser, M.; Smith, J. G., *Reagents for Organic Synthesis*, Wiley, New York, 1967 - present.

There are also some very useful organic synthesis sites in the *Synthesis and Reactions* section of the ***Organic Chemistry Directory***.

For those interested in real life organic synthesis challenges that can have financial rewards, visit:  
<http://www.innocentive.com>

**Organic Chemistry Concepts, Tutorials and Exercises.** If you would like supplements to your textbook for presentation of concepts, tutorials and additional exercises, there are many Internet sites listed in the *Educational Sites and Resources* section of the ***Organic Chemistry Directory***.

***Organic Chemistry Directory*** - <http://murov.info/orgchem.htm>