CHM 305
CHEMICAL INFORMATION RETRIEVAL AND SCIENTIFIC ETHICS

Chemical Information Resources

All citations listed below are deliberately **not** given in currently acceptable ACS format. See the "ACS Style Guide" for the format acceptable in the current ACS!

Pavia, Lampman, & Kriz (pp 787-799) has a good introductory guide to the chemical literature. Other extensive guides include the following:

1. A. Antony, "Guide to Basic Information Sources in Chemistry," Wiley, New York, 1979.
2. M. G. Mellon, "Chemical Publications - Their Nature and Use," 5th ed. McGraw-Hill, New York, 1982.
3. H. Schulz & U. Georgy, "From CA to CAS ONLINE," 2nd ed., VCH, Weinheim, 1994.
4. D.D. Ridley, "Information Retrieval: SciFinder and SciFinder Scholar," Wiley, New York 2002.
5. R. E. Maizel, "How to Find Chemical Information," 3rd ed., Wiley, New York, 1998.

Classification of Chemical Literature

I. Primary Sources

Periodicals (Journals)
Technical Reports (Government, Industry)
Patents
Dissertations

II. Secondary Sources

Periodicals (Reviews) - *Chem. Revs*., *Chem. Soc. Revs*.
Indexing Journals - *Current Contents, Chem. Titles, Sc. Cit. Index*
Abstracting Journals - *Chem. Abstr.*
Handbooks, Dictionaries, and Encyclopedias
Treatises and Monographs
Textbooks

III. Tertiary Sources

Catalogs - Aldrich, Lancaster, Strem
Trade Publications

IV. Supporting Sources

Laboratory Safety Guides
Guides to Handling Hazardous Materials
Guides to Disposal of Chemical Substances

V. CAS Online and SciFinder

Primary Sources

Primary sources are those where one finds original data. In an academic setting you will usually find original information in a journal, however other sources exist. Marshall University currently subscribes to just over 50 journals, including nearly all of the most important ones relating to the research done by faculty members here.

Some journals cover a broad array of topics. The two most important journals in this category are *Journal of the American Chemical Society* and *Angewandte Chemie*. *JACS* includes full papers and communications, while *AC* includes communications and review articles (including the Nobel Prize address in chemistry each year).

The vast majority of journals deal with either a major or minor area of chemistry. Furthermore, within a subject area with multiple periodicals there is a quality pecking order. For example, the *Journal of Organic Chemistry* (ACS) and *Perkin 1* and *Perkin 2* (RSC) are amongst the most important organic chemistry journals. The various *Tetrahedron* journals and *Synthesis*, for example, cover largely the same subject matter but are considered less prestigious.

You should realize that this does not necessarily mean their data is less accurate. In fact, the information in all of these sources is usually of comparable quality, the primary difference frequently is perceived relevance, importance, or originality. Another factor that will influence where a manuscript is published is completeness. Sometimes the nature of a study or the technology of the day precludes a definitive conclusion. Such inquiries usually are relegated to less prestigious journals.

No matter what journal you extract information from, read it critically. Ask "Does this make sense?" "Is it internally self-consistent?" For example, if you see an organic compound with a molecular weight under 100 g/mol and a melting point that says it's a solid you'd want to double check the data. Such compounds are comparatively rare. The peer review process (used in nearly all scientific publications) helps to eliminate mistakes and unwarranted claims, but mistakes still get through.

The other three primary sources include technical reports, patents, and dissertations. Technical reports generally come from government agencies and laboratories and from industry. Patents primarily come from industry but occasionally patents are obtained from academia, foundations, and individuals working at national laboratories. Dissertations are the products of students pursuing a Ph.D. degree. A requirement of doctoral programs is a written summation of the candidate's work. This work is then published in the form of a dissertation. A copy can usually be obtained from the student, his/her mentor, or UMI. UMI is a company that sells copies of all dissertations published in the United States (www.umi.com/hp/support/dservices).

Secondary Sources

Secondary sources will contain information derived from primary sources. It will be less complete than the primary source, but may nonetheless contain the information you seek. Whenever possible you should consult the primary source to verify the data you extract. Transcription errors do occur and you are responsible for them. There is more diversity of secondary sources than primary sources.

Lists of physical properties for common and not-so-common chemicals are frequently collected in handbooks, such as the *CRC Handbook of Chemistry and Physics*, *Lange's Handbook of Chemistry*, and the *Merck Index*. There are also "dictionaries" such as *Dictionary of Organic Compounds* and *Dictionary of Organometallic Compounds* that provide such data. These sources also usually provide citations to syntheses and spectroscopic data. Encyclopedias (e.g. Encyclopedia Britannica, www.britannica.com) also provide information on certain compounds and elements. In particular the *Kirk-Othmer Encyclopedia of Chemical Technology* is an enormous work on chemistry, chemical engineering, and chemical industry.

For a broad overview of the literature on a particular compound, technique, type of bonding, etc. there are two major sources. Review articles in journals and books. The major journals publishing reviews include *Accounts of Chemical Research*, *Angewandte Chemie*, *Chemical Reviews*, *Chemical Society Reviews*, *Coordination Chemistry Reviews*, and *Russian Chemical Reviews*. Of these *ACR* is different from the others. *ACR* publishes short reviews of about 5 pages written by an author primarily on his or her own work. The other review journals publish review articles substantially longer (sometimes approaching 100 pages) and are more comprehensive. All but *Coordination Chemistry Reviews* publish articles on all areas of chemistry. *Chemical Reviews* also publishes thematic issues on single subjects.

There are numerous book series in all areas of chemistry. The most general include the ACS *Advances in Chemistry* series, *Topics in Current Chemistry*, and the NATO series of books. Others deal with individual subject areas. Examples include: *Annual Review of Physical Chemistry*, *Progress in Physical Organic Chemistry*, and *Advances in Organometallic Chemistry*. There are many "Topics in," "Annual Reviews," "Progress in," and "Advances in" book series. These books contain anywhere from a 2 to 3 long reviews to a substantially larger number of shorter reviews.

Another type of reference is the book set. These sets generally use names like *Comprehensive Supramolecular Chemistry* or *Encyclopedia of Spectroscopy*. These sets will typically contain 3 – 10 volumes and will provide a broad survey of an area some, but with nowhere near the detail a typical review a journal or book will provide. They are a great place to get started.

There is probably only one chemistry abstracting service you are familiar with: *Chemical Abstracts*. *CA* began publication in 1907 and is today the premier abstracting service in chemistry. Other abstracting publications have existed (and still do). Using these sources is more important the further back in time the search goes. This is because *CA* was not as comprehensive when it began as it is today. If one wishes to search early in this century and certainly prior to the inception of *CA* one should consider *Chemisches Zentralblatt* (1830 – 1969) and *British Abstracts* (1871 – 1953).

As a general rule textbooks of the survey type are not very good sources because they contain few references. This is a reason many faculty choose books with a stronger research component for textbooks in special topics and some upper division courses. These books provide the references you will need if you use these books later in your career. They also will abstract material from several sources and synthesize them into a more coherent picture. They also have the advantage over other sources in being written with the student in mind.

Science Citation Index is a unique publication. In it one looks up a paper (paper 1) according to the author who wrote it. Entries list other papers that cite paper 1. Thus, when you find a reference that is relevant, you can look up other papers that cite it as well. This is particularly useful when trying to see how a certain bit of research was expanded upon.

Finally, there is the internet. Today, it is the first place that most people go for information much of the time because of the convenience. As you know, many primary sources are now on the internet. For example, all significant journals are now available on the internet and increasingly print copies are unavailable. The key to knowing the quality of the journal is knowing its editorial policy (e.g. is it peer reviewed or pay-to-publish) in combination to its ranking in Science Citation Index. Neither by itself ensures high quality, but in combination you can get an excellent sense of how reliable and innovative the work you are reading is. Even though it is open source, much of the information in sources like Wikipedia is reliable, but you have to read it with more care. For example, much of the general information (e.g. elemental physical properties) is undoubtedly reliable, but cutting edge information could be less so. If you plan on using information of the latter type, be sure to look at the references cited on the page and, for something important, verify it from the source. Be wary of personal webpages, although research group webpages at university websites are likely to be reasonably reliable.

Tertiary Sources

Chemical catalogues are increasingly useful sources of chemical data such as melting points and refractive indices. This largely because they are free and thus be kept in a research laboratory with little concern for their ultimate fate. Either the chemical's manufacturer or a secondary source usually provides information in catalogues. As with secondary sources, it is the responsibility of the reader to verify the accuracy of the information. Because they may well have been the source of the data, you shouldn't use secondary sources (e.g. *CRC Handbook of Chemistry and Physics*) for confirmation purposes. Material safety data sheets (MSDS) can also be used as a source of information about chemicals.