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Finding and Using Information in Analytical Chemistry

A scientist at the lab bench may work with vacuums, but no scientist works in a vacuum. Science is a cumulative process, with each experiment building on those that preceded it. A scientist must be able to determine what has already been done, how it was done, plus factual data about chemicals, procedures, instruments, and so forth. This means knowing one's way around the complex and ever-changing information universe. Learning how to find and use information is a life-long process.

This chapter is intended to give you a basic overview of chemical information and literature searching in analytical chemistry. It is intended to be general enough to be useful in any area of chemistry.

1. GETTING STARTED

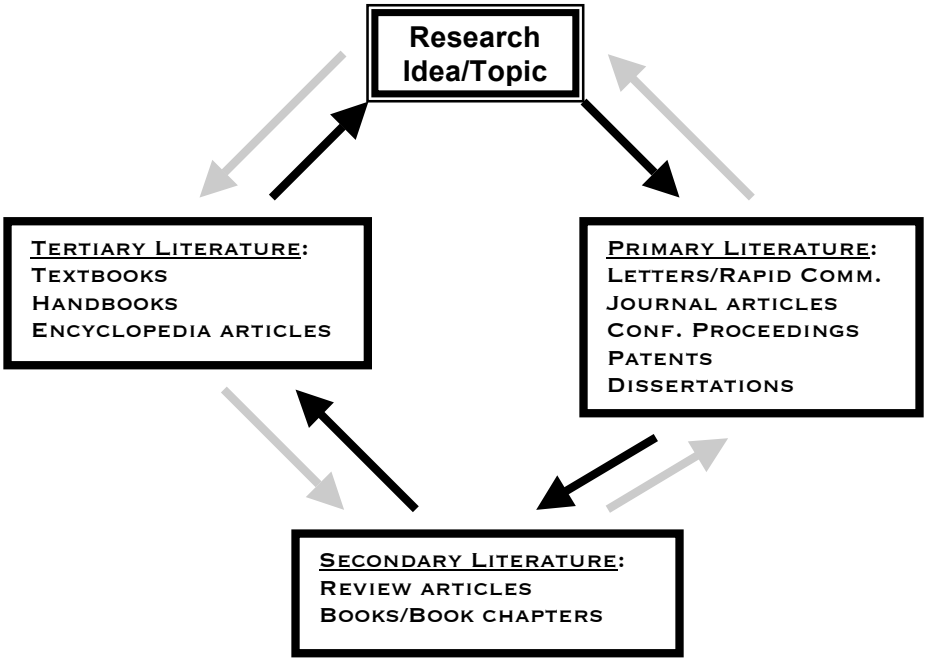
Chemistry Library
http://www.lib.utexas.edu/chem/
This is your primary portal to chemical information resources at UT Austin.

Analytical Chemistry Reference Sources
http://www.lib.utexas.edu/chem/info/analytical.html
This guide lists the most important printed reference sources in the library for analytical chemistry, chromatography, and analytical methods.

Spectra and Spectral Data Reference Sources
http://www.lib.utexas.edu/chem/info/spectra.html
This guide lists many of the most important collections of chemical spectra and spectroscopy reference materials shelved in the library's Spectra Section and on the Web.

2. THE RESEARCH-PUBLICATION CYCLE

Science is an ongoing, cyclical process that builds upon past discoveries to create new knowledge. The past informs the present, which in turn determines the future. The research-publication cycle can be thought of as a circle that moves in both directions, with one direction representing knowledge discovery and the other knowledge creation. The discovery cycle begins with an idea or topic and moves counterclockwise in the diagram: you learn about a topic by first consulting the more general, tertiary and secondary sources, then proceeding to the primary literature of journals. The Publication cycle goes in the opposite direction: new knowledge moves through the primary literature, then eventually into secondary and tertiary forms of literature.



3. TYPES OF SCIENTIFIC LITERATURE

3a. Journals

Peer-reviewed journals form the **primary literature** where new research is first reported. Scientists publish their own research in journals, and also read journals to inform their own work and to learn what others have done already. "Peer review" is a process by which a paper submitted to a journal is evaluated by experts in that field. Usually the identity of these reviewers is unknown to the author, and vice-versa, and this is called "blind peer review." Reviewers look for consistency and logic in the data, and try to spot obvious errors and conclusions that are not supported by the data. They do not edit for "style" and they usually can't detect outright fraud. Reviewers do not repeat experiments themselves, but trust the authors to have carried out stated procedures correctly and reported accurate measurements.

Many thousands of journals are currently published across all scientific and technical disciplines: Chemical Abstracts Service (CAS) scans over 9,000 of them for chemical content to index. Only a fraction of these are truly "chemistry" journals; chemical information pervades many other disciplines and CAS strives for comprehensiveness. A list of selected key journals in analytical chemistry (including spectroscopy) can be found in Appendix 1.

Journal articles fall into three basic categories. Some journals publish all types of articles, while others are devoted to only a single type.

- Full Papers

These articles describe in complete detail a specific research project or experiment, with full experimental details, results, and a conclusion. In chemistry, a full paper is usually 3-10 pages long, depending on the topic and journal. Examples of journals that publish full papers include *Analytical Chemistry, Journal of the American Chemical Society*, and *The Analyst*.

- Rapid Communications (Letters)

These are shorter papers that provide a brief summary of work in progress and report interesting preliminary results. They generally do not contain extensive experimental details or firm conclusions. As the name implies, these papers can be published much faster than full articles, which may sometimes take many months in the editorial process. The purpose of publishing rapid communications is to establish one's priority in a specific line of inquiry. Further results are usually published in full papers later on. Journals that publish mainly rapid communications include *Organic Letters, Chemical Communications*, and *Rapid Communications in Mass Spectrometry*.

- Reviews

Reviews do not report new research findings, but rather summarize and synthesize recent research on a particular topic; thus they form part of the **secondary literature**. They are a good way to introduce yourself to the journal literature on a topic, because reviews typically contain extensive bibliographies of recent and important articles. A number of journals are devoted to publishing reviews, e.g. *Chemical Reviews* and *Critical Reviews in Analytical Chemistry*.

Most journal articles are authored by teams of individuals who were involved in the research. The first author listed is usually the person who did most of the work and wrote most of the paper. That person is often also the "corresponding" author, the one to whom inquiries should be directed. The last author is usually the senior member of the research group, such as the supervising professor or lab manager. The other authors are listed in descending order of contribution. Note that in many articles the authors may not all be in one place – inter-institutional collaborations are common in the sciences. In chemistry, there are usually fewer than ten listed authors on a paper, but in other disciplines the number can be much higher.

Journal articles are written by and for specialists, not the lay person or student. They focus on a narrowly defined, specific topic. Journal space is limited, so articles do not contain much if any background information, and the authors assume a certain level of prior knowledge among their readers. So, a journal article is not the best place to start learning about a concept or procedure you're unfamiliar with. (One important exception is the *Journal of Chemical Education*, which contains articles describing experiments and concepts useful to students.)

- E-Journals vs. Print Journals

Many scientific journals are now available electronically on the Web. Most journals still publish a print version as well, but the UT Libraries now receive fewer of these. As a general rule of thumb, most scientific journals are online back to the mid-1990s. Publishers are also actively digitizing older materials. UT-Austin users have access to the American Chemical Society, Royal Society of Chemistry, and Elsevier Organic archival journal collections, which extend back into the 19th century.

While online journals are a great convenience, you must not limit yourself to reading only what is available electronically – this is irresponsible and scientifically risky. A trip to the library to look at a journal that's not online is still an important part of the research process.

- Journals vs. "Magazines"

Peer-reviewed journals form the core of the scholarly literature, but many other periodicals also exist that can be informative. Trade magazines such as *Chemical & Engineering News, LC-GC*, and *Chemical Engineering* do not contain peer-reviewed research articles and are intended for a more general audience of scientists and business people. Their content is usually authored by staff reporters and writers rather than at-large scientists, and they contain extensive advertising. Trade magazines are generally not available online except to individual subscribers, although their web sites may contain useful freely accessible content.

A hybrid well known to analytical chemists is the "A-Pages" contained within the journal *Analytical Chemistry*. The A-Pages are non-peer-reviewed magazine-style features, summary articles, news, and advertising that were (until 2006) separately paginated within the larger journal, causing much confusion for people trying to find them. The letter A appended to page numbers (e.g. 286A-289A) is the telltale sign. The A-Pages are not available in the Web archives of Analytical Chemistry before 1997, so you have to go to the printed journal to find them. In 2006 the publisher merged this content into the regular journal's pagination.

- Language

CAS indexes journals in over 50 languages. Today, over 80 percent of the non-patent chemical literature is published in English, regardless of country of origin. Nevertheless, a literature search will often reveal articles in other languages. Translations do exist for some major Russian-language journals, but otherwise you must use the original.

3b. Books

In the sciences, books (also called monographs) may be entirely written by one or more authors, but just as often they are collections of chapters by various authors assembled by an editor. Books do not report new research results; they serve instead as a summary of current knowledge and recent progress and cover a topic more broadly than journal articles do. As such they fall into the category of secondary literature, and can be regarded as reviews.

Textbooks are written specially for students, and present well-established information in a pedagogical sequence for the purposes of teaching, with plentiful illustrations, examples, and exercise questions. Some textbooks can be quite advanced, but are usually associated with undergraduate-level material.

Electronic books (e-books) have yet to catch on with readers in the way that e-journals have. E-books can be identified and accessed in the Library Catalog (see below). Only a tiny fraction of books are available as e-books. Most books are still paper objects that must be retrieved in the library.

3c. Encyclopedias

Encyclopedias, along with textbooks and handbooks, are part of the **tertiary literature**. Encyclopedia articles are written by experts and are intended for an intelligent audience of non-experts. They usually contain a bibliography for further reading. There are a number of

excellent encyclopedias covering chemistry in the library's reference collection. The titles most relevant to analytical chemistry topics are:

Encyclopedia of analytical chemistry.
Reference QD 71.5 E52 2000, 15 vols.
Extensive compilation of articles on all types of chemical analysis and instrumentation for all types of analytes and matrices. Divided into 5 volumes on Theory and Instrumentation, and 10 volumes on applications. Index in v.15.

Encyclopedia of analytical science. 2nd ed.
Reference QD 71.5 E539 2005, 10 vols.
Reference work covering all facets of analytical science in three broad areas: techniques (e.g. mass spectrometry, chromatography, etc.), areas of application (e.g. forensic, environmental, clinical); and analytes. Index in volume 10.

Encyclopedia of chromatography. 2nd ed.
Reference QD 79 C4 E63 2005 2 vols.
Articles on chromatographic techniques and applications for biotechnology, pharmacy, polymers, food additives and nutrients, pathology, toxicology, fuels, pollutants, nuclear chemistry, etc.

Encyclopedia of industrial chemical analysis.
Reference QD 131 E5, 20 vols.
Vols. 1-3 are devoted to general techniques common to many industrial products; vols. 4-19 cover analysis of specific materials. Vol. 20 is the index to vols. 4-19. Somewhat dated (1966-74), but still very useful.

Encyclopedia of separation science.
Reference QD 63 S4 E525 2000 10 vols.
Articles on the processes of any scale by which the components of a mixture are separated without substantial chemical modification. Covers areas such as affinity, centrifugation, chromatography, crystallization, distillation, electrophoresis, extraction, flotation, ion exchange, mass spectrometry, membranes and particle size. Index in volume 10.

Kirk-Othmer encyclopedia of chemical technology.
Reference TP 9 K54 2004 (5th ed.)
Core general encyclopedia focused mainly on industrial-level technology, but with a great deal of information on key chemical topics and compounds. Also available on the web.

While articles are usually arranged in an A-Z sequence, the best way to use an encyclopedia is to start with its index, found in its last volume. Only Kirk-Othmer is available online; you have to come to the library to use the print volumes of the other titles.

3d. Handbooks

Handbooks collect frequently-needed information in a concise, organized format. Some are compilations of factual data in table form. Others are more textual and summarize key techniques and methodologies. ("Handbook" is an overused term and is often found in titles that aren't really handbooks, but monographs.) Classic handbooks well known to generations of chemists include the *CRC Handbook of Chemistry and Physics* and the *Merck Index*. In

analytical chemistry you can consult *Dean's Analytical Chemistry Handbook, Handbook of Basic Tables for Chemical Analysis*, and the *Analytical Instrumentation Handbook*, among others. Use a handbook's index to look up a property name, technique, or concept.

Some of the standard handbooks such as the CRC are available in electronic format on the Web. The more specialized ones exist only in print form.

4. SEARCHING THE LITERATURE

4a. Finding Reference Books

If you need background information beyond what your textbook can tell you, try an encyclopedia. Pull one off the shelf in the library, look in its index, and scan a few articles. You'll be amazed how much you can learn this way. The bibliographies following each article are good shortcuts to the journal and book literature. Remember that most encyclopedias are printed works that must be consulted in the library – you won't be able to discover or access their contents on the Web. While encyclopedias and other reference books are listed in the Library Catalog, you generally need to find out about them by browsing the shelves in the reference collection or using a list as in Section 3c above, or a bibliography such as the Analytical Chemistry pathfinder mentioned in Section 1 above. Or just ask a librarian.

4b. Finding Books: the Library Catalog

If you need a more thorough treatment of a technique, procedure, or class of compound than an encyclopedia can offer, try finding a few books on the topic.

Search for books in the Library Catalog using keywords or known titles/authors. The Catalog URL is http://catalog.lib.utexas.edu/. A full catalog record for a book contains this kind of information:

Author Erickson, Mitchell D.
Title Analytical chemistry of PCBs / Mitchell D. Erickson.
Edition 2nd ed.
Imprint Boca Raton, FL : Lewis Publishers, 1997.
Description 667 p. : ill. ; 27 cm.
Note Originally published: Boston : Butterworth Publishers, c1986.
Bibliography Includes bibliographical references and index.
Subject Heading Polychlorinated biphenyls -- Analysis.
ISBN 0873719239
OCLC number 36670101

Location	Call Number	Current Status
Chemistry Library	QD 412 C5 E75 1997	AVAILABLE

- The Catalog indexes data from the title, author(s), and subject headings of a book. The catalog will not usually contain information on individual chapters within a book, so you

have to "think general." Don't use too many words in a catalog search query, and don't get too specialized: think about what an entire book might be about, as opposed to a more specific chapter or article. For example, you could expect to find many books on PCBs (polychlorinated biphenyls), but probably not one just about 2,4,5-trichlorobiphenyl.

- TIP: If you find a record for a book that looks relevant, open the full record and look at the SUBJECT HEADINGS assigned to that book. Clicking on one of these headings will find others with the same heading that you might not have found in your initial search.

- Note the call number and location information for books that appear promising. If a book is checked out to someone and unavailable, it will say so in the status column. You can always recall a book that is checked out, but you have to allow about a week for it to be returned.

- TIP: Once you identify a book and find it on the shelf, browse the shelves near it for other books that you might not have seen in your catalog search. Never underestimate the value of serendipity!

- Search for journals in the catalog by title or title keyword. A journal record includes a summary of the library's print holdings and locations, along with a link to the complete list of volumes, and the call number. If an electronic version is available, there should also be a link to the library's E-Journal system that will show you what parts of the journal are available to you online. *Remember that the catalog does not contain article-level information*.

- TIP: Journals for which the library has some online access but no print holdings may not be listed in the Library Catalog. In this case you should also search the e-journals database, which contains records only for journals and periodicals with electronic access. You can do this from the catalog's Journal Title search page (the second search box). http://catalog.lib.utexas.edu/screens/journaltitle.html

4c. Finding Articles: Index and Abstract Databases

Searching for the content of the journal literature (articles) is done in index databases. In chemistry, **Chemical Abstracts** (CA) is the primary indexing source. It's one of the largest and most comprehensive indexes in the world, and contains over 24 million bibliographic records back to 1907. UT students have two options for access to Chemical Abstracts:

- **Chemical Abstracts Student Edition**
  [Information: http://www.lib.utexas.edu/chem/info/castdted.html]
  CA-SE is a subset of the full Chemical Abstracts database. It includes records from about 300 core journals and annuals in chemistry, chemical engineering, polymer science, and biomedicine, back to 1967. It is Web-searchable and relatively easy to use. It is a good place to start your literature searching, because all the articles indexed are in

English, and the UT Libraries subscribe to almost all of the journals, many of them electronically. This means that you'll have access to most everything you find here.

CA-SE's interface provides you with several search boxes where you can enter keywords, and combine them using AND, OR, or NOT. If you're looking for articles describing the determination of water hardness using complexometric titration, you could enter "water hardness" in one box and "complexometric titrat*" in a second box and combine the two with the AND operator. Note the use of * to truncate the term titration to retrieve alternate forms such as "titrated" and "titrations." If you have synonyms of a particular concept, put them together in a box linked by the OR operator.

- **SciFinder**
  [Information: http://www.lib.utexas.edu/chem/scifinder.html]
  SciFinder provides network access to the suite of CAS databases with a single, user-friendly graphical interface. You can search all of Chemical Abstracts back to 1907, plus the vast Registry file of chemical substance records. In addition, Registry records link to useful information about commercial suppliers (CHEMCATS) and regulatory information (CHEMLIST), all in one place.

  SciFinder is different from most other databases in that you construct your query in natural language terms. Thus your search for water hardness would be phrased with prepositions, all on one line:
  `determination of water hardness by complexometric titration`
  SciFinder parses the query into component concepts and gives you a results selection table based on the terms' proximity in a record. Choose a results set that is focused, yet large enough to contain likely good hits.

  CAS indexes a vast array of scientific publications in all languages, including patents. You will likely run across a promising article only to discover that it's written in Chinese or Serbo-Croatian, or not available in the UT Libraries, etc. Depending on your search topic, you may also retrieve lots of patents, which generally will not be useful to you in the context of a lab course. You can refine your results to limit them to English-language and by document type.

If you're looking for a review paper, you can refine by Document Type in both SciFinder and CA-SE and select or type "Review," respectively.

Before you retrieve a full article, read its abstract first. The abstract is a brief summary of the paper's intent, methodology, and conclusions. You can usually tell from this whether the article will be of use to you, and this will save you a lot of time.

Here is a sample CA record as it appears in the Student Edition:

Author(s): Ceretti, Helena ; Hughes, Enrique A. ; Zalts, Anita
Address: Instituto de Ciencias, Area Quimica; Universidad Nacional de General Sarmiento Roca 850, San Miguel 1663, Argent.

Title: The softening of hard water and complexometric titrations: an undergraduate experiment
Source: Journal of Chemical Education 76, no. 10 (1999): 1420-1421
Additional Info: Division of Chemical Education of the American Chemical Society
Standard No: ISSN: 0021-9584 CODEN: JCEDA8
Language: English
Abstract: An undergraduate lab. expt. is described that introduces students to complexometric water hardness titrn., characteristics of an ion exchanger, and uses of an ion exchanger for water softening. The expt. is composed of a demonstration of ion-exchange properties of special resins, anal. of hard water by complexometric titrn. with EDTA, and ion-exchange softening of the water sample.
CA Section: History, Education, and Documentation 20
SUBJECT(S)
Gen Subject: Titration
>>> (complexometric; softening of hard water and complexometric titrns. as an undergraduate expt.)
Chemical education
Chemistry
Ion exchangers
Laboratory experiment
>>> (softening of hard water and complexometric titrns. as an undergraduate expt.)
Water purification
>>> (softening; softening of hard water and complexometric titrns. as an undergraduate expt.)
Identifier: undergraduate lab expt softening hard water complexometric titrn
Article Type: Journal
Accession No: CAP: 1999:616101; CAN: 131:336496

Notice that the record contains pertinent bibliographic information: the authors and the lead author's address; the title of the article and its source journal, with volume, year, and page numbers; as well as the abstract and subject headings assigned to the article by CAS for the purposes of indexing. When you do a search in the database, these are the keywords you're searching against; you're not searching the full text of the article itself.

4d. Getting Electronic Articles

Both Chemical Abstracts Student Edition and SciFinder provide links from abstracts to the online full text of articles. This way you can search the literature in one of these resources, then retrieve the full text of articles (when available) with only one or two clicks.

Within the CA-SE record you'll see a button for finding the electronic full text:

Just click this button to open up a window describing what kind of online access UT has to the article, with a link to that article if it's available. Sometimes the article is not available, and you have to go to the library to retrieve it in print. The Find it at UT window also has an option to search the library catalog just in case an electronic version isn't available.

SciFinder links work basically the same way, and takes you to a CAS site called ChemPort, which provides links both to the UT Libraries resources and directly to the publisher's site. Always prefer the UT link because we may not have access via the publisher's direct link.

4e. What About Google?

If you're a typical student you're probably accustomed to using Google, Google Scholar, or other web search engines to find things on the web, and you might call this "research." Unfortunately, if you use Google you're not really doing research at all, you're just fishing. You may find some useful things this way, but you are not doing a real literature search. Google Scholar does index an unknown portion of the scientific journal literature, but it does not do so systematically, reliably, or with any kind of expert screening. No reputable scientist can rely on this kind of searching for real work, and you shouldn't either.

4f. Why Searching Can Be Frustrating

You may have a perfectly legitimate, straightforward question in mind, the kind of question a professor or other expert could explain in a minute or two. But no such expert is available at the moment, and it's not in your textbook, so you decide to search in the literature. After a few minutes of futile searching and browsing, you realize that you're not finding the answer, and you're not sure why. Are you searching the wrong database? Are you not phrasing your query properly? Is your question too basic? It depends.

The kind of question you might have in a homework or lab assignment is generally not the kind of question for which quick answers can be found in the scientific literature. You might find things that address your question tangentially, but the journal literature is not a place where you can expect to find clear "answers" to fundamental questions. Books, particularly textbooks and encyclopedias, may be better tools for answering basic questions, but it's not often possible to search them online. Browsing a few on the library shelf is still a perfectly valid way to seek knowledge and satisfy your curiosity. Even then it may be up to you to interpret what you find and draw some conclusions on your own. That conclusion may well be "I need to get more help," and there's nothing wrong with that.

The moral of this story is that you should think about the nature of your question, then think about the best source for answering or illuminating that question. If you make a mismatch here, you'll probably wind up wasting time and not getting an answer. A giant literature database like SciFinder is often not the best place to start, so consider the other types of resources described above.

5. USING THE SCIENTIFIC LITERATURE

Finding the right information when you need it is only part of the story. After you identify and retrieve it, you have to use it! Reading a journal article and understanding what it tells you can be a challenge. Even Ph.D. chemists may have trouble comprehending the details of an article on a topic they're not fully familiar with. For students who are just learning the ropes it can be

even harder. But once you know how articles are constructed, you can locate the main points and conclusions. Remember to consult other resources such as encyclopedias for explanations of specific techniques mentioned in articles.

5a. Parts of a Paper

- Title
- Authors (with affiliations and addresses)
- Abstract (summary)
- Introduction and Literature Review
- Experimental
- Results
- Conclusion
- References

In scientific writing, brevity counts. You will notice right away that articles tend to abbreviate things, leave out what you might consider to be crucial explanations, and exclude most background detail. Authors gloss over "background" information by citing earlier articles and books, rather than repeating it. Experimental details are likewise abbreviated in a shorthand that can be mystifying to the non-specialist. With a little practice you'll be able to decipher this fairly easily.

5b. Citing Your Sources

Whenever you use data or information that you did not generate yourself from your own experimental work, and that is not considered "common knowledge in the field," you must cite your source clearly. If you do not cite a source for a statement or fact in your lab reports or research papers, you imply that you are the creator of that information, and this could get you in trouble later on. So always give credit where credit is due.

Legitimate sources to cite include:

- Journal articles
- Books and book chapters
- Conference papers
- Patents
- Handbooks
- Encyclopedias and textbooks
- *Reputable* factual databases (such as Beilstein, NIST WebBook, DIPPR, etc.)

5c. Reference Style

A journal article is routinely cited by its author(s), source, and bibliographic data (volume, year, pages). The article title is usually not given in a reference, to save space. It does not matter whether you obtained the document online or in print. It is not standard practice to provide an article's URL in a reference. URLs are not stable over time.

Follow the citation formats to journals and other types of publications as provided in Chapter 14 of the *ACS Style Guide* (3rd edition), which is available on reserve in the Chemistry Library. Some examples based on ACS styles can be found at:
http://chemistry.library.wisc.edu/writing/acs-style-guidelines.html

The actual reference format can vary slightly by journal and publisher, but in chemistry it usually follows this form:

> Smith, J.A.; Jones, P.T.; Wang, T. *J. Phys. Chem. Ref. Data* **2004**, 31, 698-710.
> [Authors in published order, last name first, first and middle intials, separated by semicolons. *Journal Title abbreviation** **Year**, *Volume*, pagination.]
>
> * Journal titles are now fully spelled out in most index databases, but are still routinely abbreviated in reference lists. Abbreviations follow certain conventions, but can sometimes be nonintuitive. If you have difficulty creating or deciphering an abbreviation, consult CASSI, which is Chemical Abstracts' cumulative listing of sources indexed since it began in 1907. CASSI is located on the Chemistry Library's circulation desk. A list of 1000 common chemistry journal abbreviations can be found in the *ACS Style Guide*.

When citing other kinds of sources, such as books, conferences, encyclopedias, databases, etc., consult the Style Guide for examples. If you use a bibliographic software such as EndNote, you can easily format your references according to a specific scholarly style.

If you wish to cite an "unpublished" source that exists only on the Web, you must of course include the source's URL, but you must be very judicious when doing this. Many editors (and professors) will reject a citation that is not to a "legitimate" source as listed above.

The goal of the reference is to provide just enough information to allow a reader anywhere to locate the document via whatever paths s/he has at his or her disposal. It is your responsibility to cite sources accurately. An incorrect citation will make it difficult if not impossible for someone to find the document. Don't assume that any citation you find in the literature is accurate – many authors are careless in this regard, and references are rarely checked in the publication process.

5d. Evaluating Information

The Web is an unstable, amorphous, disordered, and unvetted ocean of information, with a very low signal-to-noise ratio. It is a useful medium for the transfer and retrieval of published scientific information, but there is also a great deal out there that is not very reliable. For this reason it is not accepted practice to cite miscellaneous web pages as valid sources. This is because anyone can "publish" a web page saying anything at all, and alter or remove that page at any later time. Many web pages aren't attributable to a specific author or creator, and many are not dated. You have no way to verify the validity or currency of the information and no way to guarantee that future readers will be able to find it if you cite it. This includes popular resources such as Wikipedia and Answers.com, and also commercial content from instrument manufacturers and chemical suppliers.

Evaluating accuracy is a particularly important caveat in the laboratory sciences where safety is a major concern. *You should never attempt to replicate an experiment or procedure you find on a web page that cannot be firmly attributed to a reputable, reliable source.*

Not everything on the Web is dangerous or nonsensical, of course. The skills you learn as a student scientist will help you examine all resources critically, and accept some pieces of information and discard others. You should get in the habit of asking yourself questions like:

- Where does this information come from?
- Who did it? Is it signed? Is it dated?
- It is internally consistent and logical?
- Is it factual or opinion?
- Do the conclusions follow from the data?
- Is it consistent with other sources?
- Does it cite its sources?
- Is it safe?

Every piece of information you retrieve should be evaluated in this way. Naturally you're on somewhat safer ground when dealing with journal articles as opposed to miscellaneous web pages. That's not to say that journals don't sometimes publish erroneous information. No editorial and review process is perfect, and errors do occur, both in the lab and in the publishing process. Usually they're minor and don't affect the general conclusions. But sometimes the conclusions are later proven wrong – this is a natural and intentional part of the scientific process.

5e. Respecting Intellectual Property

Beyond the requirement of citing your sources properly, you must respect copyright laws when you wish to quote or reproduce content created by someone else. It is not legal to use or reproduce tables, graphics, or images from a published or unpublished source without first obtaining permission from the copyright holder. While it is rare in scientific writing to quote brief snippets of text verbatim, you may do so with proper attribution, as long as you don't quote too much.

6. OTHER TYPES OF ANALYTICAL INFORMATION

There are other types of chemical information that you might frequently need.

6a. Standard Methods of Analysis

Analytical chemists, particularly in government and industry, use collections of approved "standard methods" established by professional organizations and governmental and international agencies to test various materials for purity, composition, and contaminants. These methods are particularly relevant to the food and drug industries and to environmental regulation, and are used in the courts. The published methods are concise, and can be useful starting points for your labs. A good example is the *Official Methods of Analysis of AOAC International*, available in the Chemistry Library's reference collection (call number S 587 O38). The AOAC

(Association of Official Analytical Chemists) compiles methods related to food, foodstuffs, and drugs.

See the Analytical Chemistry pathfinder (http://www.lib.utexas.edu/chem/info/analytical.html) for a list of other methods compilations and handbooks.

6b. Sources of Chemicals

Not every chemical you might need is available in your local stockroom. It is up to you to identify the compounds you need (with instructor approval of course), and request them to be ordered. You can identify suppliers easily online using various chemical search engines or online catalogs of specific suppliers like Sigma-Aldrich and Fisher. Some catalogs and buyer's guides are listed at http://www.lib.utexas.edu/chem/info/cats.html. In SciFinder, you can search for a compound and click on the  button to access the CHEMCATS file, which is a database of chemical supplier information.

6c. Safety and Hazard Information

See the pathfinder at http://www.lib.utexas.edu/chem/info/safety.html for a list of printed reference sources on hazardous materials, toxicology, regulatory information, and laboratory safety, plus links to lists of Materials Safety Data Sheets (MSDS). In SciFinder, you can click on the  button in a compound record display to access regulatory information for that compound from the CHEMLIST.

6d. Spectroscopy and Spectra

Information about chemical spectroscopy, spectroscopic techniques, and chemical spectral data is a significant subset of the analytical chemistry literature as a whole. You can see by scanning major journals such as *Analytical Chemistry* that spectroscopy may actually dominate the field today. Monographs and textbooks focusing on various types of spectroscopy are plentiful.

Sometimes the most challenging task a researcher faces is finding a published spectrum (or spectral data) for a specific substance, or matching the spectrum of an unknown substance to that of a known substance. Computer programs and digital spectral libraries available to chemists in the lab take care of much of the latter work today. But published spectra for known compounds must usually be found in the literature. This literature falls into two types.

- 6d1. Collections of Reference Spectra

The Chemistry Library maintains a separate reference section dedicated to spectra and spectroscopy, which contains many printed collections of chemical spectra of every description. Some are very large and complex; others are compact one-volume handbooks. Encyclopedias and dictionaries are also found here. An annotated listing of the most important print and online collections and the compounds they cover can be found at this URL:

http://www.lib.utexas.edu/chem/info/spectra.html

You will note immediately that most printed collections are devoted to organic chemicals. Spectra for inorganics, polymers, drugs, and other kinds of substances do exist, but they are far fewer in number and cover a much smaller number of chemicals. A literature search is more likely to be necessary in this case. Spectra for exotic materials, or atypical kinds of spectra or wavelength ranges, may not be published at all.

One group of spectra collections that warrants specific mention here are the Sigma-Aldrich libraries of organic infrared (FT-IR) and NMR (^{1}H and ^{13}C) spectra. These are large black books shelved on the desk in the Spectra Section. They are easy to use and contain spectra for many common organic compounds as sold by Sigma-Aldrich. These spectra are also available on Sigma-Aldrich's web site in PDF form. The books are arranged by chemical class, making it a good tool to use for comparing spectra of unknowns.

- 6d2. Spectra in Journals

Chemists often report basic spectral data for newly synthesized compounds, usually in the form of UV maximum or IR/NMR peaks, in articles describing the products. However, these data are not the crux of the paper, and it is reported almost in passing, so it often is not indexed as such in Chemical Abstracts. This makes it a bit tricky to find. Also, journal editors generally prefer not to publish full spectra diagrams unless that is a major aspect of the paper; numeric data suffices and takes up less space.

SciFinder allows you to search for a chemical substance, then limit the literature retrieval to "spectral studies." This is handy, but only works for the post-1967 literature and misses most of the incidental reporting of spectral data in synthesis articles.

Appendix 1
Key Journals in Analytical Chemistry (including Spectroscopy)

- Analytical Chemistry. (the premier journal in the field)
- Analytica Chimica Acta.
- Analytical and Bioanalytical Chemistry. (formerly Fresenius Journal of Analytical Chemistry.)
- Analytical Biochemistry.
- Analytical Sciences.
- The Analyst.
- Chromatographia.
- Critical Reviews in Analytical Chemistry.
- Electrophoresis.
- Journal of AOAC International.
- Journal of Chromatographic Science.
- Journal of Chromatography A & B.
- Journal of Electroanalytical Chemistry.
- Talanta.
- TRAC - Trends in Analytical Chemistry.

Bibliography

Maizell, Robert E. *How to Find Chemical Information*. 3rd ed. (Wiley: New York, 1998)

QD 8.5 M34 1998 Reference

Skoog, Douglas A. et al. "The Literature of Analytical Chemistry." in *Fundamentals of Analytical Chemistry*. 8th ed. (Thomson Brooks/Cole, 2004), Appendix 1.
QD 75.2 S54 2004 Reserves

More Questions? Need Help?

Visit the Chemistry Library and ask for assistance: reference help is usually available weekdays before 5pm. Or, you can send email to the Ask a Librarian page at http://www.lib.utexas.edu/chem/ask.html and we will try to respond within 24 hours.

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