



Scientific Paper and Literature

Consulting the literature is an essential element of chemical research. Whether you want to confirm the identity of your latest product, or check the feasibility of an exciting new idea, it would be both unscientific and counterproductive not to conduct a thorough literature search. Moreover, it is vital to the success of your work to keep abreast of developments in chemistry in general, and in your area in particular. The problem is that finding chemical information and keeping in touch with current developments are difficult and time-consuming tasks.

Reading literature and writing scientific paper are the basic abilities as a chemist. How to find chemical information? How to write a scientific paper? This chapter is a general guide.

SECTION

1.1

Introduction to Science Paper

A research paper is a form of written academic communication which can be employed to disseminate useful information and to share academic ideas with others. Most of the research papers are written for publication in journals or conference proceedings in one's field. Publication is one of the fastest ways for propagating ideas and for professional recognition and advancement. If you have a clear idea about the features and styles of academic articles, it will be easier for you to successfully get your paper published in the target journal or accepted by an international conference.

Features of academic papers:

- The first of the features of an academic paper is the content. It is no more and no less than an objective and accurate account of a piece of research you did, either in the humanities, social, sciences, natural sciences or applied sciences. It should not be designed to teach or to provide general background.

- The second feature is the style of writing for this purpose. Your paper should contain three ingredients: precise logical structure, clear and concise language, and the specific style demanded by the journal to which it will be submitted.

- The third, which is indeed a part of the second, is the system of documenting the sources used in writing the article. At every step in the process of writing, you must take into account the ideas, facts, and opinions you have gained from

sources you have consulted.

- One of the most convenient features of academic articles is that they are divided into clearly delineated sections. This is helpful because you only have to concentrate on one section at a time. You can thus visualize more or less completely the whole paper while you are working on any part of it. Though papers of the humanities and social sciences do not always have the clearly divided sections, they share some of the common requirements with the scientific papers.

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(DOI: will be inserted by hand later)

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Photometric redshifts with the *Multilayer Perceptron* Neural Network: application to the HDF-S and SDSS

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Abstract. We present a technique for the estimation of photometric redshifts based on feed-forward neural networks. The *Multilayer Perceptron* (MLP) Artificial Neural Network is used to predict photometric redshifts in the HDF-S from an ultra deep multicolor catalog. Various possible approaches for the training of the neural network are explored, including the deepest and most complete spectroscopic redshift catalog currently available (the Hubble Deep Field North dataset) and models of the spectral energy distribution of galaxies available in

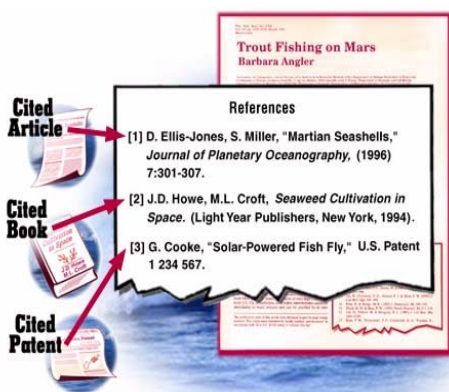
SECTION

1.2

The Structure of the Literature

Almost all chemical information is originally published in research journals, in patents, and in theses. These sources are called the primary literature and the goal of most literature searches is to find the original reports containing the required information. There are thousands of journals which publish papers on chemistry but in practice the great majority of papers which are of interest to the chemist appear in just a hundred or so of these. This is still a dauntingly large body of information but there are several routes by which it can be searched and specific items of information located.

An important route, and one which is rapid and easy, is to



tap the chemical knowledge of your colleagues and supervisors. Many of the people working around you are likely to be experts in their own fields. Another route is to use the secondary literature. This comprises review articles and books, in which the original literature has been organized and summarized, and reference books in which particular kinds of data have been collected together. Of course, finding the appropriate review or

handbook is a problem in itself. A third route is via indexes which give the literature references for all of the information on a given compound, or procedure, or author etc. prominent among these is Chemical Abstract, which contains short summaries of just about every paper published on a chemical topic, as well as comprehensive indexes to these abstracts, and hence to the original papers. Finally there are computer databases, which offer unprecedented speed, reliability, and flexibility, but at a price!

SECTION

1.3

Some Important Sources of Chemical Information

The section contains three of the most important tools for locating information in the primary literature: Chemical Abstracts, the Science Citation Index, and computer databases. It is followed by a complementary section on how to carry out some specific kinds of searches.

Chemical Abstracts

*Chemical Abstracts*TM

Your Key to the World's Chemical Literature!

CA - chemistry plus a whole lot more! Available in print and microform, CA has been alerting its subscribers to the most recent published breakthroughs in science back to the beginning of the 20th century.

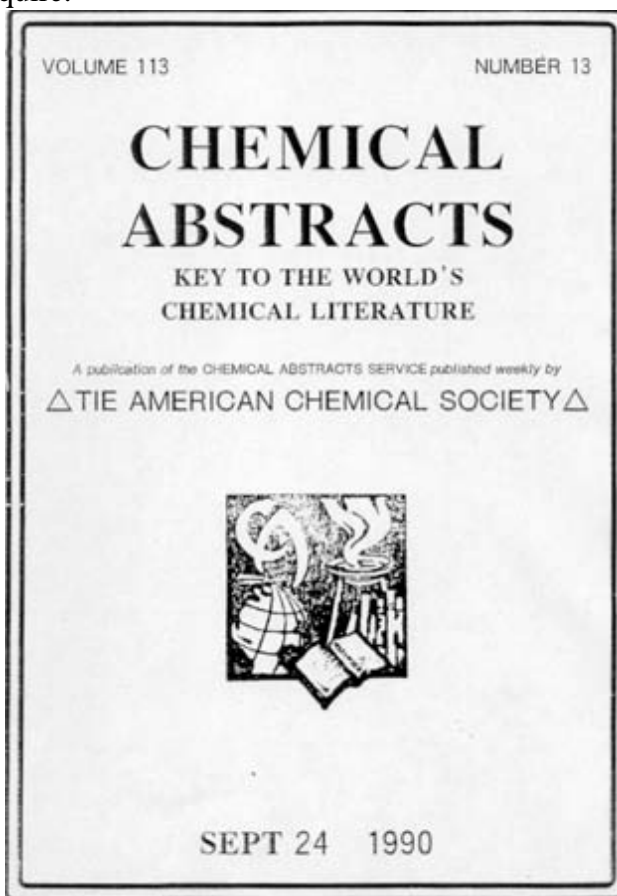
Chemical Abstracts (CA) consists two main parts, abstracts of every paper containing new chemical information, and indexes which provide access to the abstracts and then to the original literature. It is published weekly and each issue contains a keyword index, a patent index and an author index. The weekly issues are collected in volumes covering a six month period and each volume contains author, chemical substance, formula, patent and general subject indexes. Every five years the indexes for the ten volumes are combined to give Collective



Indexes. These indexes are the single most important and comprehensive information tool available to the chemist.

A search of Chemical Abstracts should begin with the appropriate index of the most recent volume and should progress backwards through the other volume until the beginning of the period covered by the most current Collective Index. The most useful indexes are the chemical substance, formula, and general subject indexes. The letters R or P before an abstract number indicate that the original work is a review or a patent respectively.

The abstracts contain full bibliographic details of the original paper, and a summary of the principal new findings reported in the paper. A glance at the abstract will tell you if the original journal is likely to be accessible, what language the paper is in, and most importantly it will give an indication of whether the paper really does contain the information you require.



<http://www.cas.org/index.html>

http://library.syr.edu/research/internet/chemistry/chemical_abstracts.html

(How to use CA)

Science Citation Index

Science Citation Index®

The *Science Citation Index* (SCI®) provides access to current and retrospective bibliographic information, author abstracts, and cited references found in 3,700 of the world's leading scholarly science and technical journals covering more than 100 disciplines. Also available is *Science Citation Index Expanded*™, which covers more than 5,800 journals. *Science Citation Index Expanded*™ can be accessed through *Web of Science*® and the online version, *SciSearch*®.



Science Citation Index (SCI) is a combination of three indexes which provide coverage of all the important publications in the physical sciences. SCI is published every two months and is cumulated annually. It includes coverage of all of the major chemistry journals.

(1) The Source Index lists the bibliographic details for the publications for each author/organization.

(2) The Permuterm Index is based on combinations of keywords in the titles of the articles published in the journals which are covered by SCI.

(3) The Citation Index is a unique feature which allows you to search the literature forward in time. The index entries are the names of the first authors of each paper which was cited in any paper published during the period covered by that issue. Its use is best illustrated with the aid of an example. Hence if you find an important paper you can use SCI to get a list of all the papers which subsequently referred to it. The drawback is that many of the references you find not be relevant to your interest and there is no way of knowing which are relevant except by consulting the Source Index, which gives the titles of the papers, or by consulting the papers themselves.

The citation index is an extremely useful tool and we recommend that you carry out a search for every key paper you come across. You can also use it to find out who is referring to your own work.

USING SCIENCE CITATION INDEX/SOCIAL SCIENCE CITATION INDEX

Science Citation Index (SCI), Social Sciences Citation Index (SSCI), and Arts & Humanities Citation Index (A&HCI), which are produced by the Institute for Scientific Information (ISI), are unique among indexes. These databases, accessed through the *Web of Science* interface, cover 1980-present and are updated every Friday. In addition to providing access to source documents like traditional indexes, they also provide access to references cited by these source documents. SCI covers journals in clinical medicine, preclinical sciences, physics, chemistry, and other sciences. SSCI covers nursing, allied health fields, education, psychology, and other social sciences.

The *Journal Citation Reports* (JCR) is a document developed from these databases and provides data such as impact factor for journals indexed by the databases. To access the JCR, accessed from the Library's web page (<http://www.utoledo.edu/library/mulford/>). Click on the **Databases by Name** link, and click on the link for **Science Citation Index**. Next, click on the **Additional Resources Tab**, then the **Journal Citation Reports** link.

<http://www.isinet.com>

<http://www.iisc.ernet.in/currsci/nov102005/1531.pdf>

<http://www.utoledo.edu/library/mulford/pdf/sci.pdf>

<http://research.ukzn.ac.za/Uploads/445603ee-6bca-4c3f-aa49-d403f1497b74/Science%20Citation%20Index%20Expanded1.pdf>

NEIWorks

Computer Databases

The development of computer databases over the last decade has brought about a revolution in the way in which we search and store chemical information. The advantages of online searching include much greater speed, greater accuracy, and greater reliability. Some computer databases include material which cannot otherwise be searched directly, e.g. the full text of many major journals and reference books, and they generally contain more information than is accessible at the majority of institutional libraries. The principal advantage is much greater flexibility and power in carrying out searches. Even more importantly it is possible to search for classes of compounds or compounds containing some specific substructure, searches which were almost impossible using printed indexes.

There are disadvantages too. Some databases do not include all of the material available in conventional form. Another problem is that the software for online searching is relatively complex, so it is more difficult to learn and, as a result, online searches by inexperienced users can be unreliable. The increasing uses of personal computers and graphical input and output have made databases searching much easier but a good understanding of the software is still essential. Finally, the cost of hardware, software, consumables, and the searches themselves, can be considerable.

It is not possible to describe the operation of the databases here because there are many chemical databases but you should get some help from your next course called Chemistry Information.

MatWeb, Your Source for Materials Information

What is MatWeb? MatWeb's [searchable database of material properties](#) includes data sheets of thermoplastic and thermoset polymers such as ABS, nylon, polycarbonate, polyester, polyethylene and polypropylene; metals such as aluminum, cobalt, copper, lead, magnesium,

nickel, steel, superalloys, titanium and zinc alloys; ceramics; plus semiconductors, fibers, and other engineering materials

We have over 65,000 materials in our database, and we are continually adding to that total to provide you with the most comprehensive free source of material property data on the web. For your convenience, MatWeb also has several [Converters and Calculators](#) that make common engineering tasks available at the click of a button. MatWeb is a work in progress. We are continually striving to find better ways to serve the engineering community. Please feel free to [contact](#) us with any comments or suggestions.

MatWeb's database is comprised primarily of data sheets and spec sheets supplied by manufacturers and distributors - let them know that you saw their material data on MatWeb.

<http://www.mateb.com/>

SECTION

1.4

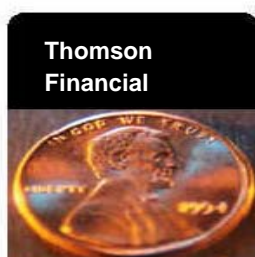
How to Find Chemical Information

The following are some basic rules for guidance in searching the literature.

- Clearly define the goals of your search.
- Discuss the problem with your colleagues and supervisors; They may have some valuable expertise.
- Decide which information source to use.
- Start with the current literature and work backwards, the recent literature will contain references to earlier work.
- When you find a key paper, check it carefully for references to relevant earlier work, and also work forward in time by carrying out a SCI search.
- Keep a complete record of your search, nothing all the sources you used and the information you obtained. This is invaluable if you have to carry out related searches later. It is advisable to keep a separate notebook for recording your literature searches, the information you accumulate will build into very useful resource.

You will know how use various tools in Chemistry Informatics.

The Thomson Corporation



SECTION

1.5

How to Start Writing?



Although there is no fixed set of “writing rules” to be followed like a cookbook recipe or an experimental procedure, some guidelines can be helpful. Start by answering some questions:

What is the function or purpose of this paper? Are you describing original and significant research results? Are you reviewing the literature? Are you providing an overview of the topic? Something else?

How is your work different from that described in other reports on the same subjects? (Unless you are writing a review, be sure that your paper will make an original contribution. Some publishers, including ACS, do not publish previously published material.)

What is the best place for this paper to be published---in a journal or as part of a book? If a journal, which journal is most appropriate?

Who is the audience? What will you need to tell them to help them understand your work?

Answering these questions will clarify your goals and thus make it easier for you to write the paper with the proper amount of detail. It will also make it easier for editors to determine the paper’s suitability for their publications. Writing is like so many other things: if you clarify your overall goal, the details fall into place.

SECTION

1.6

Components of a Paper



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Use the standard format, which is described next, for reports of original research but not necessarily for literature review or theoretical papers. Present all parts of your paper as concisely as possible.

Title

The primary aim of writing a paper is to have it read. The title is the first, and possibly the last, a reader will see of your paper. Its importance cannot be overemphasized. You must try to produce something is not only factual but stands out from the mass of other titles in the “Content” section of a journal.

The best time to determine the title is after you have written the text, so that the title will reflect the paper’s content and emphasis accurately and clearly. The title serves two main purpose: (1) to attract the potential audience and (2) to aid

retrieval and indexing. Series titles are of little value. Some publications do not permit them at all. If you cannot create a title that is short, consider breaking it into title and subtitle.

Finally, you should pay attention to the capitalization of the title you have chosen. The reason for capitalization the title are as follows:

- Capitalize the opening letter of the first word, the last word, and other important words.
- If articles, conjunctions, and prepositions don't occur in the first or last positions, they are usually left in the lower case. But prepositions of more than five letters (though, for instance) are usually capitalized.

The same rules holds for the subtitle if you choose to have one. Note that the first letter of a subtitle is also capitalized.

Authors

There are no generally accepted conventions for the order of authors if there is more than one author for one paper. Some journals require that the authors, names be listed in alphabetical order. But most journals would have them listed according to their contribution made to the research.

According to certain regulations, Chinese names in English should be spelt in pinyin with the family name first and the given name second. Capitalize the first letter of the pinyin of family name and the first letter of the first character of the given name, with the second character immediately following, without using a hyphen (-): ZHANG San.

Affiliation

The affiliation is the institution (or institutions) at which the work was conducted. If there is more than one author, use an asterisk or superscript (check the specific publication's style) to indicate the author or authors to whom correspondence should be addressed. Clarify all corresponding authors' addresses by accompanying footnotes if they are not apparent. If the current address of a corresponding author differs from that at which the work was done, give the author's current address in a footnote.

Also provide the corresponding author's e-mail address and fax number, in addition to postal address and telephone number.

Abstract

Most publications require an informative abstract for every paper, even if they do not publish abstract. An abstract is a short description, or an accurate condensation of the contents of a piece of writing.

Introduction



Have you answered these questions in your introduction?

·Have you properly oriented the reader?

·Have you told why the study (device, etc) is needed and why it is significant or unique?

·Are the scope, limitations, and problems of the study well defined?

·Does the introduction generate enough interest in the reader for him to read the entire paper?

·Is the introduction self-sufficient?

A good introduction is a clear statement of the problem or project and the reasons that you are studying it. This information should be contained in the first few sentences. Give a concise and appropriate background discussion of the problem and the significance, scope, and limits of your work. Outline what has been done before by citing truly pertinent literature, but do not include a general survey of semirelevant literature. State how your work differs from or is related to work previously published. Demonstrate the continuity from the previous work to yours. The introduction can be one or two paragraphs long. Actually, the heading "Introduction" is not used because it is superfluous; opening paragraphs are usually introductory.

Experimental Details or Theoretical Basis

In research reports, this section can also be called "Experimental Methods", "Experimental Section", or "Materials and Methods". Check the specific publication. For experimental work, give sufficient detail about your materials and methods so that other experienced workers can repeat your work and obtain comparable results. When using a standard method, cite the appropriate literature and give only the details needed.

Identify the materials used, and give information on the degree of and criteria for purity, but do not reference standard laboratory reagents. Give the chemical names of all compounds and the chemical formulas of compounds that are new or uncommon. Use meaningful nomenclature; that is, use standard systematic nomenclature where specificity and complexity require, or use trivial nomenclature where it will adequately and unambiguously define a well established compound.

Describe apparatus only if it is not standard or not commercially available. Giving a company name and model number in parentheses is nondistracting and adequate to identify established compound.

Avoid using trademarks and brand names of equipment and reagents. Use generic names; include the trademark in parentheses after the generic name only if the material or product you used is somehow different from others. Remember that trademarks often are recognized and available as such only in the country of origin.

Describe the procedures used, unless they are established and standard.

Note and emphasize any hazards, such as explosive or pyrophoric tendencies and toxicity, in a separate paragraph introduced by the word "Caution:". Include precautionary

Check the body of your paper and make sure you have answered following questions.

·Have you given necessary background material? Too much?

·Are your statements supported by facts?

·Is your paper well organized and well written in terms the reader can understand?

·Did you make a point?

handling procedures, special waste disposal procedures, and any other safety considerations in adequate detail so that workers repeating the experiments can take appropriate safety measures.

Results

Summarize the data collected and their statistical treatment. Include only relevant data, but give sufficient detail to justify your conclusions. Use equations, figures, and tables only where necessary for clarity and brevity.

Discussion

The purpose of the discussion is to interpret and compare the results. Be objective; point out the features and limitations of the work. Relate your results to current knowledge in the field and to your original purpose in undertaking the project: Have you resolved the problem? What exactly have you contributed? Briefly state the logical implications of your results. Suggest further study or applications if warranted.

Present your results and discussion either as two separate sections or as one combined section if it is more logical to do so. Do not repeat information given elsewhere in the manuscript.

Conclusions

The purpose of the conclusions section is to put the interpretation into the context of the original problem. Do not repeat discussion points or include irrelevant material. Your conclusions should be based on the evidence presented.

Summary

A summary is unnecessary in most papers. In long papers, a summary of the main points can be helpful, if you stick to the main points only. If the summary itself is too long, its purpose is defeated.

Acknowledgments

Generally, the last paragraph of the paper is the place to acknowledge people, organizations, and financing. As simply as possible, thank those person, other than coauthors, who added substantially to the work, provide advice or technical assistance, or aided materially by providing equipment or supplies. Do not include their titles. In applicable, state grant numbers and sponsors here, as well as auspices under which the work was done, including permission to publish.

References

In many journals and books, references are placed at the end of the articles or chapter; in others, they are treated as footnotes. In any case, place your list of references at the end of the manuscript. In most of journals, the style and content of references are standard regardless of where they are located.

Please answer these questions in your conclusion?

·What is the original problem?

·How is it solved?

·Has a conclusion really been made?

The accuracy of the references is the author's responsibility. If you copy citations from another source, check the original reference for accuracy and appropriate content.

Special Sections

This discussion on format applies to most manuscripts, but it is not a set of rigid rules and headings. If your paper is well organized, scientifically sound, and appropriate to the publication for which you are preparing it, you may include other sections and subsections. For example, an appendix contains material that is not critical to understanding the text but provides important background information.

Exercises

1. Look for some well-organized papers in a familiar journal in your own discipline, and study the divisions of each paper; then study the organization of each part of the main body of the paper and try to select some useful sentence patterns for each part.
2. Write a standard "Bylines" section for yourself.
3. If you are an editor or reviewer of manuscripts, what are your ethical obligations?

