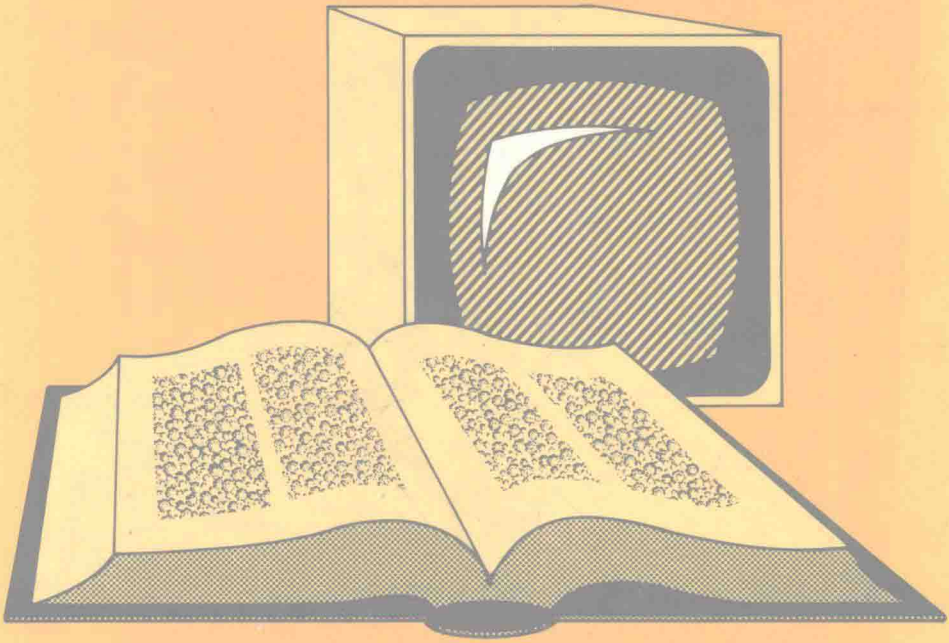
Chemical Information

A practical guide to utilization



2nd Edition

Yecheskel Wolman

CHEMICAL INFORMATION

A Practical Guide to Utilization

Second Revised and Enlarged Edition

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Preface to the Second Edition

This second edition of *Chemical Information, A Practical Guide to Utilization*, is the best demonstration of the rapid changes and developments which took place in the area of chemical information during the last five or six years. Sources that were used not long ago have been replaced by others, tools that were a must only yesterday are already forgotten today, more and more paper products are being replaced (or supplemented) by computer products. Many of today's tools will probably be changed by others in the near future.

The changes which occurred during the earlier and mid 1980s are reflected in this book. Online searching, which became a routine tool during that period, is not treated separately but is discussed through the book parallel to the various manual searching tools and sources. The basic principles and applications of expert systems, systems which are going to become more and more important in chemical information in the near future, are discussed in a separate new chapter. Another chapter is devoted to trends and perspectives in chemical information, trying to predict some of the tools and methods which will be used in the not too distant future.

Another development which took place during the early eighties is the introduction of up-to-date formal and/or informal courses in chemical information to the chemistry curricula of the undergraduate and/or graduate chemistry major students. As a matter of fact, this second edition of the book reflects the changes which took place at our teaching programme of chemical information at the Institute of Chemistry of the Hebrew University of Jerusalem.

I am indebted to my friends, colleagues and students at the Hebrew University who contributed helpful comments and remarks. Special thanks go to Ms. A. Chapman and Dr. B. A. Gore, Derwent Publication Co.; Dr. D. F. Chudos, Distributed Chemical Graphics Inc.; Ms. A. M. Cunningham, Ms. B. Lawlor and Dr. M. Main, Institute of Scientific Information; Mr. R. C. Dana, Mr. E. P. Donnell, Dr. G. P. Platau, Dr. R. Turkel and Dr. B. Zahn, Chemical Abstract Service; Dr. S. Fivozinsky, Office of Standard Reference Data, National Bureau of Standards, US Department of Commerce; Prof. E. Fluck, Director of the Gmelin Institute; Dr. S. R. Heller, USDA, ARS; Prof. R. Luckenbach, Director of the Beilstein Institute; and Mr. R. Stileman, Chapman and Hall. They provided me with an insight into their

specialities and helped me to gain a general overview of various aspects and topics of chemical information.

Yecheskel Wolman

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CHAPTER 1

Introduction

Scientists in all disciplines have the need today, more than ever, for better communication with fellow scientists. Communication is needed in order to enable one to keep up to date with the latest developments in one's field of research, to obtain specific data (e.g. chemical, biological, physical), to check the validity of a new theory, etc.

Effective and efficient communication among chemists today is possible only via an intermediate medium—the primary chemical literature (such is the case in any other area of science). Even this kind of communication, with well over 400,000 articles and about 100,000 patents published annually (not to mention other written forms: reports, deposited documents, conference abstracts and/or proceedings, theses, books), is hard to follow. It is interesting that although there are about 14,000 scientific journals that publish original chemical research results, 25% of all published articles appear in only 90 journals (e.g. in 1984 about 1800 scientific articles were published in the *Journal of the American Chemical Society*—about 0.45% of the 400,000 papers published annually), 50% in 450 journals, and 75% in 1600 journals.

In order to keep up to date in one's own field of research, and to become acquainted with new developments and trends in science, one has to cover the current literature. How can this be done? The individual chemist is not able to read all or even most of the chemical journals. Most journals today are in some specialized field, which limits the number of journals one is interested in, but nevertheless the average chemist reads a very small number of journals (usually 10–25). Some of them are of the more general type while others are in his own specific area of research. For access to news and developments not reported in these journals, the chemist refers to the secondary literature (lists of titles, abstracts, information sheets, etc.), which leads him to the original literature on topics of particular interest. But how is this done in practice?

The situation is much more complicated when one is looking for a specific data (e.g. the temperature at which the vapour pressure of ethanol is 4 atm), trying to formulate an answer based on fundamental information available (e.g. the structure–function relationship of vasopressin), or just looking for general background material in a new research area. How is the required information to be found?

All research results have been reported in the primary scientific literature (primary journals, reports, deposit documents, theses, proceedings and/or abstracts of scientific meetings, patent applications) for over 200 years. Data on the physical, biological or chemical properties of a substance, method of preparation of a compound, etc., may be used by the chemist today even if it was first reported many years ago. All that is required is that he be able to locate the required information, however long ago it was published.

An example of important available information that was difficult to locate is the data concerning the German synthetic oil programme. Although it was well known that during the Second World War the German war machine was run almost exclusively on coal-derived gasoline, there was no reference to the German technology in the scientific literature for over three decades. This was not because of lack of documentary information; plant diagrams (at the end of the War 25 oil-from-coal plants existed), patents, data on the catalysts and additives used, as well as environmental controls data were available. The problem was that the information was not reported in any of the common sources and was difficult to locate.

Correct usage of the chemical literature and other available information sources requires considerable effort. However, the benefits gained by correct usage make these extra efforts worth while.

There are a large number of books devoted to the chemical literature and its usage, and a few should be mentioned:

H.M. Woodburn, *Using the Chemical Literature. A Practical Guide*, Marcel Dekker, New York, 1974, 302pp.

R.T. Bottle (Editor), *Use of Chemical Literature*, 3rd ed., Butterworths, London, 1979, 320pp.

A. Antony, *Guide to Basic Information Sources in Chemistry*, Jeffrey Norton Publishers, New York, 1979, 219pp.

H. Skolnik, *The Literature Matrix of Chemistry*, Wiley-Interscience, New York, 1982, 297pp.

M.G. Mellon, *Chemical Publications, Their Nature and Use*, 5th ed. McGraw-Hill, New York, 1982, 395pp.

J. Ash, P. Chubb, S. Ward, S. Welford and P. Willett, *Communication, Storage and Retrieval of Chemical Information*, Ellis Horwood, Chichester, 1985, 297pp.

R.E. Maizel, *How to Find Chemical Information. A Guide for Practicing Chemists, Educators and Students*, 2nd ed., Wiley-Interscience, New York, 1986, 412pp.

These books include discussion of primary and secondary sources. Some concentrate more heavily on the various references tools, such as abstracts, indexes, handbooks and dictionaries, whereas others put the emphasis on the various types of primary literature—journals, reports, theses, and patents.

Some are more comprehensive than others but none emphasize real search problems and their solutions.

This book is intended to teach and demonstrate the practical use of the chemical literature. It will show and teach the chemist (whether he is a graduate or an undergraduate student, or whether he is dealing with academic or industrial research, scientific administration, sales, teaching or consulting) how to keep up to date in his own area of interest and will show him the best way to locate any information he requires using various paper, microform and electronic tools and products. This will be done by giving real search examples from various areas of chemistry. Some of the information could be located by using well known sources, whereas the remainder could be found by other means. The different ways of obtaining the required data will be compared and the various means and methods used for the purpose will be critically evaluated.

CHAPTER 2

The Scientific Journal

The scientific article is and will be (at least for the foreseeable future) the most important and essential document to scientists, as it is the basic unit of the scientific journal. The scientific journal itself is public, formal, and the most organized channel of communication among the scientific community. It is public as anybody can submit a manuscript to a scientific journal, and the journal itself is available to anyone either by personal subscription or through the library. It is formal as articles are examined, reviewed and (if there is a need) revised to near perfection. The organization is based on the acceptance of articles on the basis of their scientific merits; thus those articles report flawlessly research results which are a part of the scientific progress.

The formal as well as the organizational aspects of the scientific journal are taken care of by fellow scientists (peer review). This is understandable, as only people that have proven themselves in their scientific discipline could judge and decide about the novelty, quality and importance of a contribution to this specific field.

2.1. The scientific article

There are four types of journal articles—a full paper, a note (or a short paper), a communication (known also as a preliminary communication or a letter to the editor), and a review.

A full paper presents new important data or provides a new and fresh approach to an established subject. It usually consists of an informative, concise abstract, which summarizes the principle findings of the work, an introduction, which clearly states the problems, the background of the work and the approach of the author, a detail experimental section, which gives information about materials and non-standard apparatus used and a full description of how the work was done, a summary of the results, and a discussion of their significance. A note or a short paper is of course shorter than a full paper and describes more limited findings. Notes usually do not have an abstract—the emphasis is on the experimental section, while the introduction, results and discussion are short. Communications are preliminary reports of results of special significance and urgency that are given

expedited publication. They consist mainly of results and discussion sections and have only a very short introduction and minimum experimental data; some communications are followed later by a full paper. The authors often have to justify the submission of a scientific contribution for publication as a preliminary communication in a covering letter to the journal editor. Review articles usually do not contain new experimental results nor experimental details (reviews published in *Synthesis* or *Organic Reactions* are among the exceptions and do contain a few experimental examples). Reviews do correlate and integrate results, relevant to the subject in question, from various publications. One of the most important functions of a review is to serve as a guide to the original literature. When conducting a retrospective search, it is advisable first to examine reviews dealing with the subject before reading the original papers. Reviews can be divided into three categories. First, a comprehensive coverage of the subject up to the time of writing (e.g. *Chemical Reviews*, *Organic Reactions*); second, coverage of a subject for a limited period of time, usually a year or two [e.g. *The Specialist Periodical Reports Series* published by The Royal Society of Chemistry (RSC) (formerly the Chemical Society)]; and third, reviews written by people working intensively in the field and whose contribution to it is well recognized, and in which the emphasis is on the author's own views and contributions (e.g. *Accounts of Chemical Research*). Reviews are published not only in journals but also in a large number of serials prefixed by: *Progress in...*, *Advances in...*, *Fortschritte...*, etc., as well as by other serial publications (e.g. *Organic Reactions*, *Survey of Progress in Chemistry*, *Topics in Current Chemistry*).

Very few journals publish all four types of articles. Few publish three types (e.g. *Journal of Medicinal Chemistry* and *Journal of Organic Chemistry* publish full papers, notes, and communications). Some publish only papers and do not differentiate between a full paper and a note (e.g. *Journal of the Chemical Society Perkin Transactions I* and *II*), whereas others publish only full papers and communications (e.g. *Journal of the American Chemical Society*). There are journals that publish only communications (e.g. *Journal of the Chemical Society Chemical Communications*, *Tetrahedron Letter*). Some journals publish review articles and notes (e.g. *Synthesis*, *Angewadte Chemie*) while others publish reviews and papers without differentiation between a full paper and a note (e.g. *Tetrahedron*).

2.2. Publication of scientific journals

Who publishes the scientific journals and what are the publishers' interest in their publication?

One of the main functions of a scientific society is the provision of good scientific journals. Indeed, most of the prestige journals are published by scientific societies. The American Chemical Society (ACS) publishes 22 high-quality journals (Table 2.1); furthermore, the Chemical Abstract Service

Table 2.1 Journals published by the ACS

Accounts of Chemical Research
Analytical Chemistry
Biochemistry
Chemical Reviews
Chemical and Engineering News
Chemtech
Energy and Fuels
Environmental Science and Technology
Industrial and Engineering Chemistry
InorganicChemistry
Journal of the American Chemical Society
Journal of Chemical and Engineering Data
Journal of Chemical Education
Journal of Chemical Information and Computer Science
Journal of Medicinal Chemistry
Journal of Organic Chemistry
Journal of Physical Chemistry
Journal of Physical and Chemical Reference Data
Langmuir
Macromolecules
Organometallics

(CAS) which is the publisher of *Chemical Abstracts* (*CA*) is a division of the American Chemical Society.

Among the various activities of governmental agencies dealing with research and development, the publication of primary scientific journals is included, e.g. the National Research Council of Canada (NRCC) is the publisher of 12 scientific journals (Table 2.2), 6 of which are of interest to chemists.

Table 2.2 Journals published by the NRCC

Canadian Geotechnical Journal
Canadian Journal of Biochemistry and Cell Biology
Canadian Journal of Botany
Canadian Journal of Chemistry
Canadian Journal of Civil Engineering
Canadian Journal of Earth Science
Canadian Journal of Forest Research
Canadian Journal of Genetics and Cytology
Canadian Journal of Microbiology
Canadian Journal of Physics
Canadian Journal of Physiology and Pharmacology
Canadian Journal of Zoology

Publishing scientific journals is still a profitable business today, and indeed various commercial publishing houses publish a large number of journals in various fields of science (e.g. natural sciences, medicine, social sciences).