

The Literature of Organic Chemistry

All discoveries in the laboratory must be published somewhere if the information is to be made generally available. A new experimental result that is not published might as well not have been obtained, insofar as it benefits the entire chemical world. The total body of chemical knowledge (called *the literature*) is located on the combined shelves of all the chemical libraries in the world. Anyone who wishes to learn whether the answer to any chemical question is known, and, if so, what the answer is, has only to turn to the contents of these shelves. Indeed, the very expressions “is known,” “has been done,” and so on, really mean “has been published.” To the uninitiated, the contents of the shelves may appear formidably large, but fortunately the process of extracting information from the literature of organic chemistry is usually not difficult. In this appendix, we will examine the literature of organic chemistry.¹ It is quite clear that The Literature can be divided into two broad categories: primary sources and secondary sources. A *primary source* publishes the original results of laboratory investigations. Books, indexes, and other publications that cover material that has previously been published in primary sources are called *secondary sources*. It is because of the excellence of the secondary sources in organic chemistry (especially *Chemical Abstracts*TM, SciFinder[®], and Beilstein) that literature searching is comparatively not difficult. The two chief kinds of primary source are journals and patents. There are several types of secondary source.

¹For books on the chemical literature, see Wolman, Y. *Chemical Information*, 2nd ed., Wiley, NY, 1988; Maizell, R.E. *How to Find Chemical Information*, 2nd ed., Wiley, NY, 1987; Mellon, M.G. *Chemical Publications*, 5th ed., McGraw-Hill, NY, 1982; Skolnik, H. *The Literature Matrix of Chemistry*, Wiley, NY, 1982; Antony, A. *Guide to Basic Information Sources in Chemistry*, Jeffrey Norton Publishers, NY, 1979; Bottle, R.T. *Use of the Chemical Literature*, Butterworth, London, 1979; Woodburn, H.M. *Using the Chemical Literature*, Marcel Dekker, NY, 1974. For a three-part article on the literature of organic chemistry, see Hancock, J.E.H. *J. Chem. Educ.* 1968, 45, 193–199, 260–266, 336–339.

PRIMARY SOURCES

Journals

For well over 100 years, nearly all new work in organic chemistry (except for that disclosed in patents) has been published in journals. There are thousands of journals that publish chemical papers, in many countries and in many languages. Some print papers covering all fields of science; some are restricted to chemistry; some to organic chemistry; and some are still more specialized. Fortunately for the sanity of organic chemists, the vast majority of important papers in “pure” organic chemistry (as opposed to “applied”) are published in relatively few journals, perhaps 50 or fewer. The concept of “pure” organic chemistry is not as useful because organic chemistry is now important in many areas. Literature that is important to an organic chemist is found in journals and patents that focus on bioorganic, organometallic, materials science, separation science, medicinal chemistry, pharmaceutical sciences, and medicine to name a few. The reader is therefore cautioned that the journals listed in this section have organic chemistry as their primary focus, but are by no means the only sources of information concerning organic chemistry. The literature is vast and many journals are published weekly, and some semi-monthly.

In addition to ordinary papers, there are two other types of publications in which original work is reported: *notes* and *communications*. A note is a brief paper, often without a summary (nearly all papers are published with summaries or abstracts prepared by the author). Otherwise, a note is similar to a paper.² Communications (also called *letters*) are also brief and usually without summaries (though some journals now publish summaries along with their communications, a welcome trend). However, communications differ from notes and papers in three respects:

1. They are brief, not because the work is of small scope, but because they are condensed. Usually, they include only the most important experimental details or none at all.
2. They are often of immediate significance. Journals that publish communications make every effort to have them appear as soon as possible after they are received. Some papers and notes are of great importance, and some are of lesser importance, but all communications are supposed to be of high importance. With modern computer technology, communications can often be published in a matter of weeks, and the on-line version (e.g., the American Chemical Society ASAP papers) can be found before the print version appears.
3. Communications are preliminary reports, and the material in them may be republished as papers at a later date, in contrast to the material in papers and notes, which cannot be republished.

²In some journals, notes are called “short communications,” an unfortunate practice, because they are not communications as that term is defined in the text.

Although papers (we use the term in its general sense, to cover notes and communications also) are published in many languages, the English-speaking chemist is in a fairly fortunate position. At present well over half of the important papers in organic chemistry are published in English. Not only are American, British, and British Commonwealth journals published almost entirely in English, but so are many others around the world. There are predominantly English-language journals published in Japan, Italy, Czechoslovakia, Sweden, The Netherlands, Israel, and other countries. In a reorganization, six prominent European journals (*Chemische Berichte*, *Liebigs Annalen der Chemie*, *Bulletin de la Société Chimique de France*, *Bulletin des Sociétés Chimique Belges*, *Recueil des Travaux Chimiques des Pays-Bas*, and *Gazzetta Chimica Italiana*) have been discontinued. In their place is the *European Journal of Organic Chemistry*, published in English. Most of the articles published in other languages have summaries printed in English also. For many years, the second most important language (in terms of the number of organic chemical papers published) was Russian, and most of these papers are available in English translation, although in most cases, 6 months to 1 year later. With the political changes in Russia, however, many of these Journals have been modified or discontinued. Important papers have been published in German and French for >200 years, and these are generally not available in translation, so that the organic chemist should have at least a reading knowledge of these languages. In recent years, however, fewer papers in French or German have appeared without an English translation, such as in the journal *Angewandte Chemie*, which in 1962 became available in English under the title *Angewandte Chemie International Edition in English*. Of course, a reading knowledge of French and German (especially German) is critical for the older literature. Before ~1920, more than one-half of the important chemical papers were in these languages. It must be realized that the original literature is never obsolete. With the rise of China in the scientific community, journals are published in Chinese, and there are journals published in Japanese. Work by Chinese and Japanese scientists regularly appears in English-language journals, however. Secondary sources become superseded or outdated, but nineteenth century journals are found in most chemical libraries and are still consulted. Table A.1 presents a list of the more important current journals that publish original papers³ and communications in organic chemistry. Some of them also publish review articles, book reviews, and other material. Changes in journal title have not been infrequent; footnotes to the table indicate some of the more important, but some of the other journals listed have also undergone title changes. In 1999, the *Journal of Organic Chemistry* stopped publishing communications, and these are now published in a new journal, *Organic Letters*.

The primary literature has grown so much in recent years that attempts have been made to reduce the volume. One such attempt is the *Journal of Chemical Research*, begun in 1977. The main section of this journal, called the "Synopsis," publishes synopses, which are essentially long abstracts, with references. The full texts of most of the papers are published only in microfiche and miniprint versions.

³In Table A.1, notes are counted as papers.

TABLE A.1. A List of the More Important *Current Journals That Currently Publish Original Papers in Organic Chemistry*^a

No.	Name	Papers or Communications	Issues per Year
1	Angewandte Chemie (1887) ⁴	C ⁵	12
2	Angewandte Chemie International Edition (1962) ⁶	C ⁷	48
3	Australian Journal of Chemistry (1948)	P	12
4	Bioorganic Chemistry (1971)	P ⁵	4
5	Bioorganic & Medicinal Chemistry Letters (1991)	C	12
6	Bulletin of the Chemical Society of Japan (1926)	P	12
7	Canadian Journal of Chemistry (1929)	P,C	12
8	Carbohydrate Research (1965)	P,C	22
9	Chemistry, a European Journal (1995)	P	24
10	Chemistry, an Asian Journal (2006)	New	New
11	Chemistry and Industry (London) (1923)	C	24
12	Chemistry Letters (1972)	C	12
13	Chimia (1947)	C ⁵	12
14	Collection of Czechoslovak Chemical Communications (1929)	P	12
15	Doklady Chemistry (1922) ⁴	C	12
17	European Journal of Organic Chemistry (1998)	P	12
18	Helvetica Chimica Acta (1918)	P	8
19	Heteroatom Chemistry (1990)	P	6
20	Heterocycles (1973)	C ⁵	12
21	Indian Journal of Chemistry (Section B)	P	12
22	International Journal of chemical Kinetics (1969)	P	12
23	Israel Journal of Chemistry (1963)	P ⁸	4
23	Journal of the American Chemical Society (1879)	P,C	52
25	Journal of Carbohydrate Chemistry (1981)	P,C	6
26	Journal of Chemical Research, Synopses (1977)	P	12
27	Chemical Communications (1965)	C	24
28	Journal of Combinatorial Chemistry (2000)	P,C	6
29	Journal of Computational Chemistry (1979)	P	16
30	Journal of Fluorine Chemistry (1971)	P,C	12

⁴These journals are available in English translation.⁵These journals also publish review articles regularly.⁶These journals are available in English translation.⁷These journals also publish review articles regularly.⁸Each issue of this journal is devoted to a specific topic.

TABLE A.1 (Continued)

No.	Name	Papers or Communications	Issues per Year
31	Journal of Heterocyclic Chemistry (1964)	P,C	12
32	Journal of the Indian Chemical Society (1924)	P	12
33	Journal of Lipid Research (1959)	P	12
34	Journal of Medicinal Chemistry (1958)	P,C	12
35	Journal of Molecular Structure (1967)	P,C	16
36	Journal of Organometallic Chemistry (1963)	P,C	48
37	Journal of Organic Chemistry (1936)	P,C	26
38	Journal of Photochemistry and Photobiology, A: Chemistry (1972)	P	12
39	Journal of Physical Organic Chemistry (1988)	P	12
40	Journal of Polymer Science Part A (1962)	P	24
41	Journal für Praktische Chemie (1834)	P	6
42	Macromolecules (1968)	P,C	26
43	Liebigs Annalen der Chemie (1832)	P	12
44	Mendeleev Communications (1991)	C	8
45	Monatshefte für Chemie (1870)	P	12
46	New Journal of Chemistry (1977) ⁹	P	11
47	Organometallics (1982)	P,C	12
48	Organic and Biomolecular Chemistry (2003)	P	24
49	Organic Letters (1999)	C	12
50	Organic Mass Spectrometry (1968)	PC	12
51	Organic Preparations and Procedures International (1969)	P ⁵	6
52	Organic Process Research & Development (1997)	P	6
53	Photochemistry and Photobiology (1962)	P ⁵	12
54	Polish Journal of Chemistry (1921) ⁹	PC	12
55	Pure and Applied Chemistry (1960)	¹⁰	12
56	Research on Chemical Intermediates (1973) ¹¹	P ⁵	6
57	Russian Journal of Organic Chemistry (1984)	P,C	12
58	Sulfur Letters (1982)	C	6
59	Synlett (1989)	C ⁵	12
60	Synthetic Communications (1971)	C	22
61	Synthesis (1969)	P ⁵	12
62	Tetrahedron (1958)	P ⁵	52
63	Tetrahedron: Asymmetry (1990)	PC	12
64	Tetrahedron Letters (1959)	C	52

^aThese Journals are listed in alphabetical order of *Chemical Abstracts*TM abbreviations, Which Are Indicated in Boldface. Also given are the year of founding, number of issues per year as of 1998, and whether the journal primarily publishes papers (P), communications (C), or both.

⁹Before 1978 this journal was called *Roczniki Chemii*.

¹⁰*Pure Appl. Chem.* publishes IUPAC reports and lectures given at IUPAC meetings.

¹¹Before 1989 this journal was called *Reviews of Chemical Intermediates*.

For some years, the American Chemical Society journals, including *J. Am. Chem. Soc.* and *J. Org. Chem.*, have provided supplementary material for some of their papers. This material is available on-line, and for older literature from the Microforms and Back Issues Office at the ACS Washington, DC, office, either on microfiche or as a photocopy. Many other journals now offer supplementary material, generally experimental procedures, supporting spectral data and crystallographic data. These practices have not yet succeeded in substantially reducing the total volume of the world's primary chemical literature.

Patents

In many countries, including the United States, it is possible to patent a new compound or a new method for making a known compound (either laboratory or industrial procedures), as long as the compounds are useful. It comes as a surprise to many to learn that a substantial proportion of the patents granted (perhaps 20–30%) have been chemical patents. Chemical patents are part of the chemical literature, and both U.S. and foreign patents are regularly abstracted by *Chemical Abstracts*TM. In addition to learning about the contents of patents from this source, chemists may consult the *Official Gazette* of the U.S. Patent Office, which, published weekly and available in many libraries, lists titles of all patents issued that week. Bound volumes of all U.S. patents are kept in a number of large libraries, including the New York Public Library, which also has an extensive collection of foreign patents. Photocopies of any U.S. patent and most foreign patents can be obtained at low cost from the U.S. Patent and Trademark Office, Washington, DC, 20231. Many patents can now be obtained on-line as well. In addition, *Chemical Abstracts*TM lists, in the introduction to the first issue of each volume, instructions for obtaining patents from 26 countries. Patents are also available via SciFinder[®].

Although patents are often very useful to the laboratory chemist, and no literature search is complete that neglects relevant patents, as a rule they are not as reliable as papers. There are two reasons for this:

1. It is in the interest of the inventor to claim as much as possible. Therefore, they may, for example, actually have carried out a reaction with ethanol and with 1-propanol, but will claim all primary alcohols, and perhaps even secondary and tertiary alcohols, glycols, and phenols. An investigator repeating the reaction on an alcohol that the inventor did not use may find that the reaction gives no yield at all. In general, it is safest to duplicate the actual examples given, of which most chemical patents contain one or more.
2. Although legally a patent gives an inventor a monopoly, any alleged infringements must be protected in court, and this may cost a good deal of money. Therefore some patents are written so that certain essential details are concealed or entirely omitted. This practice is not exactly cricket, because a patent is supposed to be a full disclosure, but patent attorneys are generally

skilled in the art of writing patents, and procedures given are not always sufficient to duplicate the results.

Fortunately, the above statements do not apply to all chemical patents: many make full disclosures and claim only what was actually done. It must also be pointed out that it is not always possible to duplicate the work reported in every paper in a journal due to the use of proprietary catalysts, equipment, or procedures. Note, however, that some work is not published or patented, but rather maintained within the company as a trade secret. Such work is not, of course, available to the public.

SECONDARY SOURCES

Journal articles and patents contain virtually all of the original work in organic chemistry. However, if there were no indexes, abstracts, review articles, and other secondary sources, the literature would be unusable, because it is so vast that no one could hope to find anything in particular. Fortunately, the secondary sources are excellent. There are various kinds and the categories tend to merge. Our classification is somewhat arbitrary.

Listings of Titles

The profusion of original papers is so great that publications that merely list the titles of current papers find much use. Such lists are primarily methods of alerting the chemist to useful papers published in journals that they do not normally read. This approach, using print versions containing lists or journals and articles, is not used much nowadays. Most journals are available on-line, and many have the original papers, with supplemental material, as HTML and pdf¹² documents. The pdf document can be downloaded to the searcher's desktop, usually for a fee, and is most convenient. *Chemical Abstracts*TM was originally available on-line as *CAS ONLINE*. *CAS ONLINE* was discontinued when *STN*[®] (a service that CAS operates in cooperation with the German organization FIZ Karlsruhe, see below) was introduced in 1984. All of the *Chemical Abstracts*TM literature can be accessed using CAS databases online. Many libraries and companies pay the appropriate fees, so accessing the journals is usually quite easy via those organizations. Search engines allow one to quickly scan an enormous amount of literature from office or home. In addition, most browsers have on-line searching capabilities via various search engines, and simply typing in an author, a topic, a chemical, or a few key words can lead to important articles or information. Some of the important on-line technology will be discussed below. However, some of the available resources¹³ include Specialty Citation Indexes, Science Citation Index ExpandedTM, Web of Science[®],

¹²Adobe Acrobat[®] files.

¹³See <http://scientific.thomson.com/products/categories/citation/>

Science Citation Index[®], ISI ProceedingsSM, Reaction Citation Index[™], and the Derwent Innovations IndexSM. Science Citation Index[®] is available on STN[®], where it is called SciSearch. We will begin with the older print-versions for chemical searches.

A print-version “title” publication covering the whole of chemistry is *Current Contents Physical, Chemical & Earth Sciences*,¹⁴ which began in 1967 and appears weekly, contains the contents pages of all issues of ~800 journals in chemistry, physics, earth sciences, mathematics, and allied sciences. Each issue contains an index of important words taken from the titles of the papers listed in that issue, and an author index, which, however, lists only the first-named author of each paper. The author’s address is also given, so that one may write for reprints. An on-line service is available called Current Contents Connect[®] is a multidisciplinary Web resource providing access to complete bibliographic information from >8000 of the world’s leading scholarly journals and >2000 books.¹⁵

CAS databases on-line described below allows one to search a variety of databases, including journal titles.

Abstracts

Listings of titles are valuable, as far as they go, but they do not tell what is in the paper, beyond the implications carried by the titles. Most current journals contain a graphic abstract as well as a title and a brief print description of the research. The graphical abstract is extremely useful for scanning the literature presented in a journal, and both the print and graphical abstracts are available on-line for most journals.

From the earliest days of organic chemistry, abstracts of papers have been widely available, often as sections of journals whose principal interests lay elsewhere.¹⁶ At the present time there are only two publications entirely devoted to abstracts covering the whole field of chemistry. One of these, *Referativnyi Zhurnal, Khimiya*, which began in 1953, is published in Russian and is chiefly of interest to Russian-speaking chemists. The other is *Chemical Abstracts*[™] (CA). This publication, which appears weekly, prints abstracts in English of virtually every paper containing original work in pure or applied chemistry published anywhere in the world.¹⁷ More than 9500 currently published journals are covered, in many languages. In addition, CA publishes abstracts of every patent of chemical interest from 50 national and international patent offices. *Chemical Abstracts*[™] lists and indexes, but does not abstract review articles and books. The abstracts currently appear in 80 sections, of which sections 21–34 are devoted to organic chemistry, under such

¹⁴Title pages of organic chemistry journals are also carried by *Current Contents Life Sciences*, which is a similar publication covering biochemistry and medicine.

¹⁵<http://scientific.thomson.com/products/cccl/>

¹⁶For example, *Chem. Ind. (London)* publishes abstracts of papers that appear in other journals. In the past, journals, such as *J. Am. Chem. Soc.*, *J. Chem. Soc.*, and *Berchti* also did so.

¹⁷For a guide to the use of CA, see Schulz, H. *From CA to CAS ONLINE*; VCH: NY, 1988.

headings as Alicyclic Compounds, Alkaloids, Physical Organic Chemistry, Heterocyclic Compounds (One Heteroatom), and so on. Each abstract of a paper begins with a heading that gives (1) the abstract number;¹⁸ (2) the title of the paper; (3) the authors' names as fully as given in the paper; (4) the authors' address; (5) the abbreviated name of the journal (see Table A.1);¹⁹ (6) the year, volume, issue, and page numbers; and (7) the language of the paper. In earlier years, *CA* gave the language only if it differed from the language of the journal title. Abstracts of patents begin with the abstract number, title, inventor and company (if any), patent number, patent class number, date patent issued, country of priority, patent application number, date patent applied for, and number of pages in the patent. The body of the abstract is a concise summary of the information in the paper. For many common journals the author's summary (if there is one) is used in *CA* as it appears in the original paper, with perhaps some editing and additional information. Each issue of *CA* contains an author index, a patent index, and an index of keywords taken from the titles and the texts or contexts of the abstracts. The patent index lists all patents in order of number. The same compound or method is often patented in several countries. *Chemical Abstracts* will abstract only the first patent, but it does list the patent numbers of the duplicated patents in the patent index along with all previous patent numbers that correspond to it. Before 1981, there were separate Patent Number Indexes and Patent Concordances (the latter began in 1963).

At the end of each section of *CA*, there is a list of cross-references to related papers in other sections.

*Chemical Abstracts*TM is, of course, highly used for "current awareness"; it allows one to read, in one place, abstracts of virtually all new work in chemistry, though its large size puts a limit on the extent of this type of usefulness.²⁰ *Chemical Abstracts*TM is even more useful as a repository of chemical information, a place for finding out what was done in the past. This value stems from the excellent indexes, which enable the chemist in most cases to ascertain quickly where information is located. From the time of its founding in 1907 until 1961, *CA* published annual indexes. Since 1962 there are two volumes published each year, and a separate index is issued for each volume. For each volume there is an index of subjects, authors, formulas, and patent numbers. Beginning in 1972, the subject index has been issued in two parts, a chemical substance index and a general subject index, which includes all entries that are not the names of single chemical substances. However, the indexes to each volume become essentially superseded as collective indexes are issued. The first collective indexes are 10-year (decennial) indexes, but the volume of information has made 5-year indexes necessary since 1956. Collective indexes published to date are shown in Table A.2. Thus a user of the indexes at the time of this writing would consult the collective indexes through 1995 and the semiannual indexes thereafter. The 14th collective index (covering

¹⁸Beginning in 1967. See p. 1880.

¹⁹These abbreviations are changed from time to time. Therefore the reader may notice inconsistencies.

²⁰It is possible to subscribe to *CA Selects*, which provides copies of all abstracts within various narrow fields, such as organofluorine chemistry, organic reaction mechanisms, and organic stereochemistry.

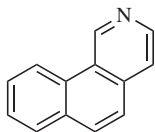
TABLE A.2. CA Collective Indexes Published

Collective Index	Subject and General Subject	Chemical Substance	Author	Formula	Patent
1	1907–1916		1907–1916		
2	1917–1926		1917–1926		1907–1936
3	1927–1936		1927–1936	1920–1946	
4	1937–1946		1937–1946		1937–1946
5	1947–1956		1947–1956	1947–1956	1947–1956
6	1957–1961		1957–1961	1957–1961	1957–1961
7	1962–1966		1962–1966	1962–1966	1962–1966
8	1967–1971		1967–1971	1967–1971	1967–1971
9	1972–1976	1972–1976	1972–1976	1972–1976	1972–1976
10	1977–1981	1977–1981	1977–1981	1977–1981	1977–1981
11	1982–1986	1982–1986	1982–1986	1982–1986	1982–1986
12	1987–1991	1987–1991	1987–1991	1987–1991	1987–1991
13	1992–1996	1992–1996	1992–1996	1992–1996	1992–1996
14	1997–2001	1997–2001	1997–2001	1997–2001	1997–2001
15	2002–2006	2002–2006	2002–2006	2002–2006	2002–2006

1997–2001) appeared in 2002. The 15th Collective index will be issued only in CD ROM, as well as any subsequent collective, presumably.

Beginning with the eighth collective index period, *CA* has published an *Index Guide*. This publication gives structural formulas and/or alternate names for thousands of compounds, as well as many other cross-references. It is designed to help the user efficiently and rapidly to find *CA* references to subjects of interest in the general subject, formula, and chemical substance indexes. Each collective index contains its own *Index Guide*. A new *Index Guide* is issued every 18 months. The *Index Guide* is necessary because the *CA* general subject index is a “controlled index,” meaning it restricts its entries only to certain terms. For example, anyone who looks for the term “refraction” in the general subject index will not find it. The *Index Guide* includes this term, and directs the reader to “Electromagnetic wave, refraction of,” “Sound and ultrasound, refraction of,” and other terms, all of which will be found in the general subject index. Similarly, the chemical substance index usually lists a compound only under one name, the approved *CA* name. Trivial and other names will be found in the *Index Guide*. For example, the term “methyl carbonate” is not in the chemical substance index, but the *Index Guide* does have this term, and tells us to look for it in the chemical substance index under the headings “carbonic acid, esters, dimethyl ester” (for Me_2CO_3) and “carbonic acid, esters, monomethyl ester” (for MeHCO_3). Furthermore, the *Index Guide* gives terms related to the chosen term, helping users to broaden a search. For example, one who looks for “Atomic orbital” in the *Index Guide* will find the terms “Energy Level,” “Molecular orbital,” “Atomic integral,” and “Exchange, quantum mechanical, integrals for,” all of which are controlled index terms.

Along with each index (annual, semiannual, or collective) appears an index of ring systems. This valuable index enables the user to ascertain immediately if any ring system appears in the corresponding subject or chemical substance index and under what names. For example, someone wishing to determine whether any compounds containing this ring system

Benz(*h*)isoquinoline

are reported in the 1982–1986 collective index (even if they did not know the name) would locate, under the heading “3-ring systems,” the listing **6, 6, 6** (since the compound has three rings of six members each), under which they would find the sub-listing C₅N–C₆–C₆ (since one ring contains five carbons and a nitrogen while the others are all-carbon), under which is listed the name benz(*h*)isoquinoline, as well as the names of 30 other systems C₅N–C₆–C₆. A search of the chemical substance index under these names will give all references to these ring systems that appeared in *CA* from 1982 to 1986.

Before 1967, *CA* used a two-column page, with each column separately numbered. A row of letters from *a* to *h* appeared down the center of the page. These letters are for the guidance of the user. Thus an entry 7337*b* refers to the *b* section of column 7337. In early years, superscript numbers (e.g., 4327⁵), were used in a similar manner. In very early years, these numbers were not printed on the page at all, though they are given in the decennial indexes, so that the user must mentally divide the page into nine parts. Beginning with 1967, abstracts are individually numbered and column numbers are discarded. Therefore, beginning with 1967, index entries give abstract number rather than column number. The abstract numbers are followed by a letter that serves as a check character to prevent miscopying errors in computer handling. To use the *CA* general subject, chemical substance, and formula indexes intelligently requires practice, and the student should become familiar with representative volumes of these indexes and with the introductory sections to them, as well as with the *Index Guides*.

In the *CA* formula indexes, formulas are listed in order of (1) number of carbon atoms; (2) number of hydrogen atoms; (3) other elements in alphabetic order. Thus, all C₃ compounds are listed before any C₄ compound; all C₅H₇ compounds before any C₅H₈ compound; C₇H₁₁Br before C₇H₁₁N; C₉H₆N₄S before C₉H₆O, and so on. Deuterium and tritium are represented by D and T and treated alphabetically, for example, C₂H₅DO after C₂H₅Cl and before C₂H₅F or C₂H₆.

Since 1965, *CA* has assigned a Registry Number to each unique chemical substance; CAS Registry Number[®]. This is a number of the form [766-51-8] that remains invariant, no matter what names are used in the literature. More than

10 million numbers have already been assigned and thousands are added each week. At one time, all numbers published with the *CA* preferred names appeared in a multivolume "Registry Handbook," but this work was discontinued. The CAS Registry contains >27 million organic and inorganic substances and >57 million sequences.²¹ For a discussion of online searching see pp. 1901–1905.

There were a number of earlier abstracting publications now defunct. The most important are *Chemisches Zentralblatt* and *British Abstracts*. These publications are still valuable because they began before *CA* and can therefore supply abstracts for papers that appeared before 1907. Furthermore, even for papers published after 1907, *Zentralblatt* and *British Abstracts* are often more detailed. *Zentralblatt* was published, under various names, from 1830 to 1969.²² *British Abstracts* was a separate publication from 1926 to 1953, but earlier abstracts from this source are available in the *Journal of the Chemical Society* from 1871 to 1925.

Beilstein

This publication is so important to organic chemistry that it deserves a section by itself. Beilstein's *Handbuch der Organischen Chemie*, usually referred to as *Beilstein*, lists all the known organic compounds reported in the literature during its period of coverage. We will first describe the print version, particularly important for older literature. This discussion will be followed by a description of the on-line version of Beilstein – Crossfire Beilstein. For each compound are given: all names; the molecular formula; the structural formula; all methods of preparation (briefly, e.g., "by refluxing 1-butanol with NaBr and sulfuric acid"); physical constants, such as melting point and refractive index; other physical properties; chemical properties including reactions; occurrence in nature (i.e., which species it was isolated from); biological properties, if any; derivatives with melting points; analytical data, and any other information that has been reported in the literature.²³ Equally important, for every piece of information, a reference is given to the original literature. Furthermore, the data in *Beilstein* have been critically evaluated. That is, all information is carefully researched and documented, and duplicate and erroneous results are eliminated. Some compounds are discussed in two or three lines and others require several pages. The value of such a work should be obvious.

The first three editions of *Beilstein* are obsolete. The fourth edition (*vierte Auflage*) covers the literature from its beginnings through 1909. This edition, called *das Hauptwerk*, consists of 27 volumes. The compounds are arranged in order of a

²¹This total is updated daily. See <http://www.cas.org/cgi-bin/regreport.pl>.

²²An "obituary" of *Zentralblatt* by Weiske, which gives its history and statistical data about its abstracts and indexes, was published in the April 1973 issue of *Chem. Ber.* (pp. I–XVI).

²³For a discussion of how data are processed for inclusion in *Beilstein*, see Luckenbach, R.; Ecker, R.; Sunkel, J. *Angew. Chem. Int. Ed.* **1981**, *20*, 841.

system too elaborate to discuss fully here.²⁴ The compounds are divided into three divisions that are further subdivided into “systems”:

Division	Volumes	System Numbers
I. Acyclic Compounds	1–4	1–499
II. Carbocyclic Compounds	5–16	450–2359
III. Heterocyclic Compounds	17–27	2360–4720

Das Hauptwerk is still the basis of *Beilstein* and has not been superseded. The later literature is covered by supplements that have been arranged to parallel *das Hauptwerk*. The same system is used, so that the compounds are treated in the same order. The first supplement (*erstes Ergänzungswerk*) covers 1910–1919; the second supplement (*zweites Ergänzungswerk*) covers 1920–1929; the third supplement (*drittes Ergänzungswerk*) covers 1930–1949; the fourth supplement (*viertes Ergänzungswerk*) covers 1950–1959, and the fifth supplement covers 1960–1979. Like *das Hauptwerk*, each supplement contains 27 volumes,²⁵ except that supplements 3 and 4 are combined for Vols. 17–27, so that for these volumes the combined third and fourth supplement covers the years 1930–1959. Each supplement has been divided into volumes in the same way as *das Hauptwerk*, and, for example, compounds found in Vol. 3, system number 199 of *das Hauptwerk* will also be found in Vol. 3, system number 199 of each supplement. To make cross-referencing even easier, each supplement gives, for each compound, the page numbers at which the same compound can be found in the earlier books. Thus, on page 554 of Vol. 6 of the fourth supplement, under the listing phenetole are found the symbols (H 140; E I 80; E II 142; E III 545) indicating that earlier information on phenetole is given on page 140 of Vol. 6 of *das Hauptwerk*, on page 80 of the first, page 142 of the second, and page 545 of the third supplement. Furthermore, each page of the supplements contains, at the top center, the corresponding page numbers of *das Hauptwerk*. Since the same systematic order is followed in all six series, location of a compound in any one series gives its location in the other five. If a compound is found, for example, in Vol. 5 of *das Hauptwerk*, one has but to note the page number and scan Vol. 5 of each supplement until that number appears in the top center of the page (the same number often covers several pages). Of course, many compounds are found in only one, two, three, four, or five of the series, since no work may have been published on that compound during a

²⁴For descriptions of the *Beilstein* system and directions for using it, see Sunkel, J.; Hoffmann, E.; Luckenbach, R. *J. Chem. Educ.* **1981**, *58*, 982; Luckenbach, R. *CHEMTECH* **1979**, 612. The Beilstein Institute has also published two English-language guides to the system. One, available free, is *How to Use Beilstein*; Beilstein Institute: Frankfurt/Main, **1979**. The other is by Weissbach, O. *A Manual for the Use of Beilstein's Handbuch der Organischen Chemie*, Springer, NY, **1976**. An older work, which many students will find easier to follow, is by Huntress, E.H. *A Brief Introduction to the Use of Beilstein's Handbuch der Organischen Chemie*, 2nd ed., Wiley, NY, **1938**.

²⁵In some cases, to keep the system parallel and to avoid books that are too big or too small, volumes are issued in two or more parts, and, in other cases, two volumes are bound as one.

particular period covered. From *das Hauptwerk* to the fourth supplement, *Beilstein* is in German, though it is not difficult to read since most of the words are the names of compounds (a *Beilstein* German–English Dictionary, available free from the publisher, is in many libraries). For the fifth supplement (covering 1960–1979), which is in English, publication of Division III began before the earlier divisions. At the time of this writing, Vols. 17–22 (totaling 70 separate parts exclusive of index volumes) of this supplement have been published, as well as a combined index for Volumes 17–19. This index covers only the fifth supplement. The subject portion of this index, which lists compound names only, gives these names in English.

Volumes 28 and 29 of *Beilstein* are subject and formula indexes, respectively. The most recent complete edition of these volumes is part of the second supplement and covers only *das Hauptwerk* and the first two supplements (though complete indexes covering *das Hauptwerk* and the first four supplements have been announced to appear in the next few years). For Vol. 1, there is a cumulative subject and a cumulative formula index, which combine *das Hauptwerk* and the first four supplements.²⁶ Similar index volumes, covering all four supplements, have been issued for the other volumes, 2–27. Some of these are combined (e.g., 2–3, 12–14, and 23–25). For English-speaking chemists (and probably for many German-speaking chemists) the formula indexes are more convenient. Of course (except for the fifth supplement indexes), one must still know some German, because most formula listings contain the names of many isomers. If a compound is found only in *das Hauptwerk*, the index listing is merely the volume and page numbers (e.g., 1, 501). Roman numbers are used to indicate the supplements, for example, 26, 15, I 5, II 7. Thus the subject and formula indexes lead at once to locations in *das Hauptwerk* and the first four supplements. The *Beilstein* formula indexes are constructed the same way as the *CA* indexes (p. 1880).

There is also a fourth division of *Beilstein* (systems 4721–4877) that covers natural products of uncertain structure: rubbers, sugars, and so on. These are treated in Vols. 30 and 31, which do not go beyond 1935, and which are covered in the collective indexes. These volumes will not be updated. All such compounds are now included in the regular *Beilstein* volumes.

Like *CA*, *Beilstein* is available on-line, with the useful search engine *CrossFire Beilstein*. The *Beilstein* database is one of the best databases for organic chemistry, particularly synthetic organic chemistry. It contains information on ~9.4 million organic substances that have been fully characterized, as well as 9.8 million reactions. Information available includes:²⁷

- Structure and reaction diagrams
- Identification information (name, formula, registry numbers, etc.)

²⁶Most page number entries in the combined indexes contain a letter, for example, CHBr₂Cl 67f, II 33a, III 87d, IV, 81. These letters tell where on the page to find the compound and are useful because the names given in the index are not necessarily those used in the earlier series. The letter “a” means the compound is the first on its page, “b” is the second, and so on. No letters are given for the fourth supplement.

²⁷<http://gethelp.library.upenn.edu/guides/tutorials/scitech/beilstein/BCWhat.html>

- Isolation and purification information
- Derivatives
- Physical properties, including
- Structure and energy parameters
- State of matter and change of state information
- Transport phenomena
- Optical properties
- Spectra (UV, VIS, MS, NMR, IR, ESR, X-ray, etc.)
- Electrical and magnetic properties
- Electrochemistry
- Behavior of liquid/solid, liquid/liquid, and liquid/vapor systems
- Solution behavior
- Energy data
- Optical data
- Boundary surface phenomena
- Adsorption
- Association
- Pharmacological and ecological data

Not all compounds contain all different types of data. Some data, often those quantities that can be described by a number, word, or short phrase, are given explicitly in the record for the compound. Others simply have a literature reference. The factual data, of which there are 260 million, are only experimental data, scientifically measured.

Coverage of the Literature and Search Capabilities

Beilstein references the chemical literature published in ~175 prestigious organic chemistry journals²⁸ from 1771 to date. It is updated quarterly. The database may be searched using structures and/or text (property information, chemical name, molecular formula).” Figure A. 1 shows the on-line page after a structure has been drawn using the drawing tools provided with the program, used by Crossfire to begin a session. Figure A. 2 shows an on-line page that displays data obtained after a structure search. The variety of tools available for searching is much more extensive than the ones shown in Figs. A.1 and A.2. One can use the structure editor to draw a specific structure, and it is possible to draw two or more structures, label them as reactant and/or product and search for a chemical reactions or transformation. A variety of data can be accessed for a compound or a reaction, and the output includes the chemical structures, references to the primary literature, physical, and spectral properties where available.

²⁸See <http://www.mdl.com/products/pdfs/BSJournals.pdf>.

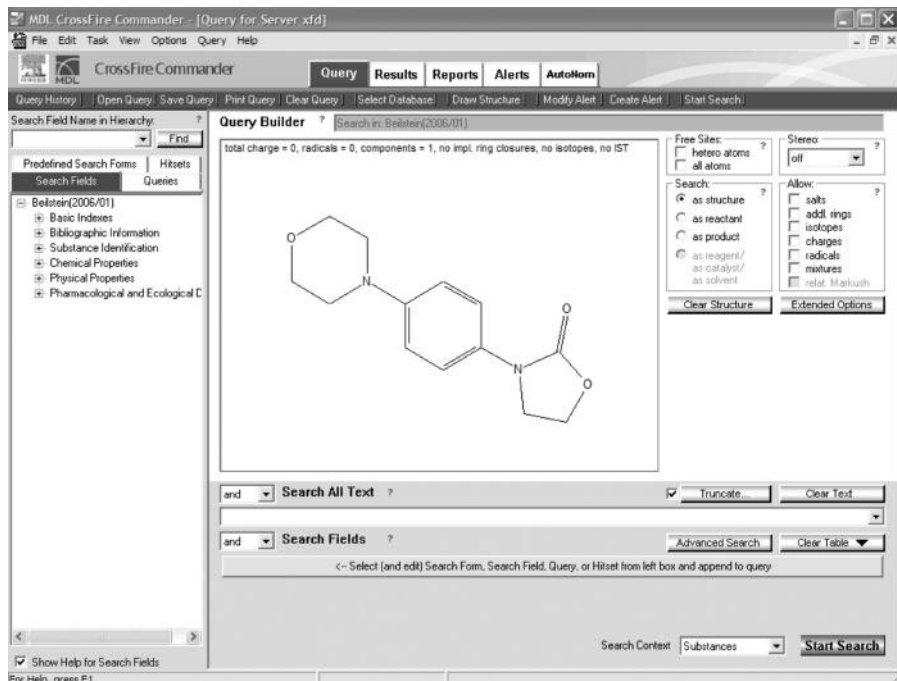


Fig. A.1. Structure Search for CrossFire Beilstein²⁹ Beilstein Data: Copyright (c) 1988–2006, Beilstein Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH. All rights reserved.

Tables of Information

In addition to *Beilstein*, there are many other reference works in organic chemistry that are essentially compilations of data. These books are very useful and often save the research worker a great deal of time. In this section we discuss some of the more important of such works.

1. The sixth edition of *Heilbron's Dictionary of Organic Compounds*, J. Buckingham, Ed., 9 vols., Chapman and Hall, London, **1996**, contains brief listings of >150,000 organic compounds, giving names, structural formulas, physical properties, and derivatives, with references. For many entries additional data concerning occurrence, biological activity, and toxicity hazard information are also given. The arrangement is alphabetical. The dictionary contains indexes of names, formulas, heteroatoms, and CA Registry Numbers. Annual supplements, with cumulative indexes, have appeared since 1983. A similar work, devoted to organometallic compounds, is the 2nd edition of the *Dictionary of Organometallic Compounds*, 6 vols. in its 5th supplement,

²⁹See http://www.mdl.com/products/knowledge/crossfire_commander/.

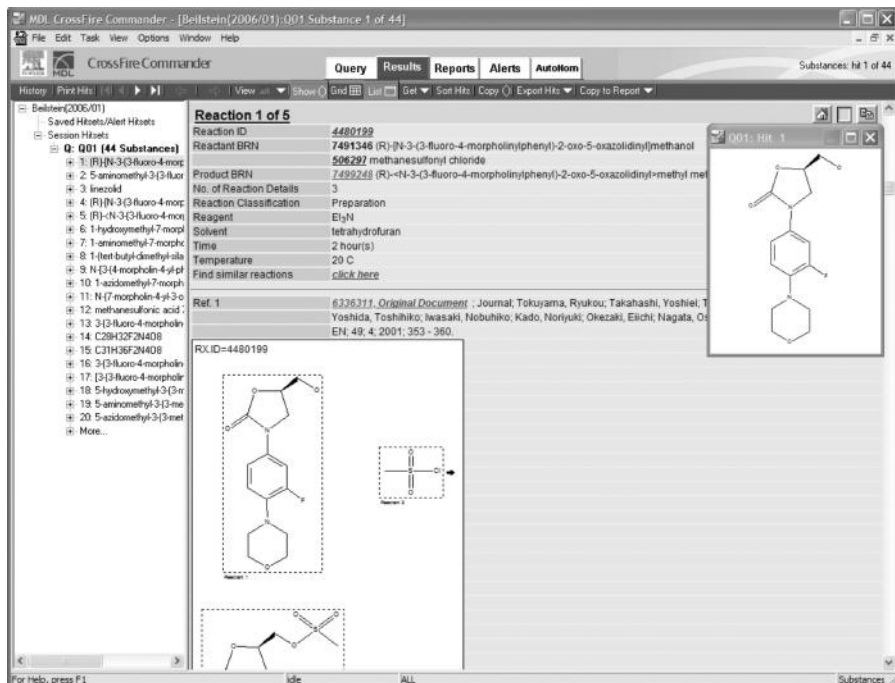


Fig. A.2. Preparation Data from CrossFire Beilstein.³⁰ Beilstein Data: Copyright (c) 1988–2006, Beilstein Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH. All rights reserved.

published by Chapman and Hall in **1989**. Another, *Dictionary of Steroids*, 2 vols., 1991, is also published by Chapman and Hall.

2. A multivolume compendium of physical data is Landolt-Börnstein's *Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik, und Technik*, 6th ed., Springer, Berlin, **1950**–. There is also a “New Series,” for which the volumes are given the English title *Numerical Data and Functional Relationships in Science and Technology*, as well as the German title. This compendium, which is not yet complete, lists a great deal of data, some of which are of interest to organic chemists (e.g., indexes of refraction, heats of combustion, optical rotations, and spectral data). Literature references are given for all data.
3. *The Handbook of Chemistry and Physics*, CRC Press, Boca Raton, FL (called the “rubber handbook”), which is revised annually (87th ed., **2006–2007**), is a valuable repository of data quickly found. For organic chemists the most important table is “Physical Constants of Organic Compounds,”

³⁰See http://www.mdl.com/products/knowledge/crossfire_beilstein/index.jsp. Also see, <http://chemistry.library.wisc.edu/beilstein/quickguide6.htm>

which lists names, formulas, color, solubilities, and physical properties of thousands of compounds. However, there are many other useful tables. A similar work is *Lange's Handbook of Chemistry*, 16th ed., McGraw-Hill, New York, **2004**. Another such handbook, but restricted to data of interest to organic chemists, is *Dean's Handbook of Organic Chemistry*, 2nd ed., McGraw-Hill, New York, **2003**. This book also contains a long table of "Physical Constants of Organic Compounds," and has much other information including tables of thermodynamic properties, spectral peaks, pK_a values, bond distances, and dipole moments.

4. A list of most of the known natural compounds (e.g., terpenes, alkaloids, carbohydrates), to which structures have been assigned, along with structural formulas, melting points, optical rotations, and references, is provided in Devon and Scott, *Handbook of Naturally Occurring Compounds*, 3 vols., Academic Press, New York, **1972**.
5. Dreisbach, *Physical Properties of Chemical Compounds*, Advances in Chemistry Series Nos. 15, 22, 29, American Chemical Society, Washington, DC, **1955–1961** lists many physical properties of >1000 organic compounds.
6. Physical properties of thousands of organometallic compounds, with references, are collected in five large compendia: the *Dictionary of Organometallic Compounds*, mentioned under item 1, above; Dub, *Organometallic Compounds*, 2nd ed., 3 vols. with supplements and index, Springer, New York, **1966–1975**; Hagihara, Kumada, and Okawara, *Handbook of Organometallic Compounds*, W. A. Benjamin, New York, 1968; and Kaufman, *Handbook of Organometallic Compounds*, Van Nostrand, Princeton, NJ, 1961; *Comprehensive Organometallic Chemistry II*, 14 Vols, Pergamon, 1995.
7. The *Merck Index*, 13th ed., Merck and Company, Rahway, NJ, **2001** is a good source of information about chemicals of medicinal importance. Many drugs are given three types of name: chemical name (which is the name an organic chemist would give it; of course, there may well be more than one); generic name, which must be placed on all containers of the drug; and trade names, which are different for each company that markets the drug. For example, the generic name for 1-(4-chlorobenzhydryl)-4-methylpiperazine is chlorcyclazine. Among the trade names for this drug, which is an antihistamine, are Trihistan, Perazyl, and Alergicide. The *Merck Index* is especially valuable because it gives all known names of all three types for each compound and the names are cross-indexed. Also given, for each compound, are the structural formula, CA preferred name and Registry Number, physical properties, medicinal and other uses, toxicity indications, and references to methods of synthesis. There are indexes of formulas and Registry Numbers, and miscellaneous tables. The 10th edition of the *Merck Index* (1983) also includes a lengthy list of organic name reactions, with references. Although the 11th edition omitted this list, it was restored in the 12th and subsequent editions.

Note that the Merck Index Online™ is also available.

8. There are two publications that list properties of azeotropic mixtures. Timmermans, *The Physicochemical Constants of Binary Systems in Concentrated Solutions*, 4 vols., Interscience, New York, **1959–1960**, is by far the more comprehensive. The other is *Azeotropic Data*, 2 vols., Advances in Chemistry Series Nos. 6 and 35, American chemical Society, Washington, DC, **1952, 1962**.
9. Thousands of dipole moments, with references, are collected in McClellan, *Tables of Experimental Dipole Moments*, Vol. 1, W.H. Freeman, San Francisco, CA, **1963**; Vol. 2, Raha Enterprises, El Cerrita, CA, **1974**.
10. *Tables of Interatomic Distances and Configurations in Molecules and Ions*, London chemical Society Special publication No. 11, 1958, and its supplement, Special publication No. 18, **1965**, include bond distances and angles for hundreds of compounds, along with references.
11. The *Ring Systems Handbook*, published in **1988** by the Chemical Abstracts Service, provides the names and formulas of ring and cage systems that have been published in *CA*. The ring systems are listed under a system essentially the same as that used for the *CA* index of ring systems (p. \$\$\$). Each entry gives the *CA* index name and Registry Number for that ring system. In many cases, a *CA* reference is also given. There is a separate Formula Index (for the parent ring systems) and a Ring Name Index. Cumulative supplements are issued twice a year. The *Ring Systems Handbook* supersedes earlier publications called *The Parent Compound Handbook* and *The Ring Index*.
12. The Sadtler Research Laboratories publish large collections of IR, UV, NMR and other spectra, in loose-leaf form. Indexes are available.
13. Infrared, UV, NMR, Raman, and mass spectral data, as well as melting-point, boiling-point, solubility, density, and other data for >30,000 organic compounds are collected in the *CRC Handbook of Data on Organic Compounds*, 2nd ed., 9 vols., CRC Press, Boca Raton, FL, **1988**, edited by Weast and Grasselli. It differs from the Sadtler collection in that the data are given in tabular form (lists of peaks) rather than reproduction of the actual spectra, but this book has the advantage that all the spectral and physical data for a given compound appear at one place. References are given to the Sadtler and other collections of spectra. Volumes 7–9 contain indexes of spectral peaks for IR, UV, ^1H NMR, ^{13}C NMR, mass, and Raman spectra, as well as indexes of other names, molecular formulas, molecular weights, and physical constants. Annual updates began appearing in **1990** (the first one is called Vol. 10).
14. The *Aldrich Library of Infrared Spectra*, 3rd ed., Aldrich chemical Company, Milwaukee, WI, **1981**, by Pouchert contains >12,000 IR spectra so arranged that the user can readily see the change that takes place in a given spectrum when a slight change is made in the structure of a molecule. The same company also publishes the *Aldrich Library of FT-IR Spectra* and the *Aldrich Library of NMR Spectra*, both also by Pouchert. A similar volume, which has IR and Raman spectra of ~1000 compounds, is *Raman/Infrared Atlas of Organic Compounds*, 2nd ed., VCH, New York, **1989**, by Schrader.

15. An extensive list of visible and UV peaks is given in *Organic Electronic Spectral Data*, Wiley, New York. Twenty-six volumes have appeared so far, covering the literature through 1984.
16. A collection of 500 ^{13}C NMR spectra is found in Johnson and Jankowski, *Carbon-13 NMR Spectra*, Wiley, New York, 1972.

Reviews

A review article is an intensive survey of a rather narrow field; for example, the titles of some recent reviews are “Desulfonation Reactions: Recent Developments,”³¹ “Pyrrolizidine and Indolizidine Syntheses Involving 1,3-Dipolar Cycloaddition,”³² and “From Corrin Chemistry to Asymmetry Catalysis—A Personal Account.”³³ A good review article is of enormous value, because it is a thorough survey of all the work done in the field under discussion. Review articles are printed in review journals and in certain books. The most important review journals in organic chemistry (though most are not exclusively devoted to organic chemistry) are shown in Table A.3. Some of the journals listed in Table A.1, for

TABLE A.3. Review Journals, With Year of Founding and Issues per Year as of 1998

Journal	Issues
Accounts of Chemical Research (1968)	12
Aldrichimica Acta (1968)	4
Angewandte Chemie (1888) and its English Translation: Angewandte Chemie, International Edition (1962)	12
Chemical Reviews (1924)	8
Chemical Society Reviews (1947) ³⁴	4
Heterocycles (1973)	12
Natural Product Reports (1984)	6
Organic Preparations and Procedures International (1969)	6
Soviet Scientific Reviews, Section B , Chemistry Reviews (1979) Irreg.	
Sulfur Reports (1980)	6
Synlett (1989)	12
Synthesis (1969)	12
Tetrahedron (1958)	52
Topics in Current Chemistry (1949) ³⁵	Irreg.
Uspekhi Khimii (1932) and its English translation: Russian chemical Reviews (1960)	12

³¹Nájera, C.; Yus, M. *Tetrahedron* **1999**, 55, 10547.

³²Broggini, G.; Zecchi, G. *Synthesis* **1999**, 905.

³³Pfaltz, A. *Synlett* **1999**, 835.

³⁴Successor to *Quarterly Reviews* (abbreviated as *Q. Rev., Chem. Soc.*).

³⁵Formerly called *Fortschritte der Chemischen Forschung*.

example, *Synlett*, *Tetrahedron*, *Synthesis*, *Organic Preparations and Procedures International*, and *J. Organomet. Chem.* also publish occasional review articles.

There are several open-ended serial publications that are similar in content to the review journals, but are published irregularly (seldom more often than once a year) and are hardbound. Some of these publish reviews in all fields of chemistry; some cover only organic chemistry; some specialize further. The coverage is indicated by the titles. Table A.4 shows some of the more important such publications, with *CA* abbreviations.

There are several publications that provide listings of review articles in organic chemistry. The most important is the *J. Org. Chem.*, which began to list review articles in 1978 (the first list is at *J. Org. Chem.*, 43, 3085), suspended the listings in 1985, and resumed them in 1990 (at *J. Org. Chem.*, 55, 398). These lists, which appear about four times a year, give the titles and reference sources of virtually

TABLE A.4. Irregularly Published Serial Publications

Advances in Carbocation Chemistry
Advances in Carbohydrate Chemistry and Biochemistry
Advances in Catalysis
Advances in Cycloaddition
Advances in Free Radical Chemistry
Advances in Heterocyclic Chemistry
Advances in Metal-Organic Chemistry
Advances in Molecular Modeling
Advances in Organometallic Chemistry
Advances in Oxygenated Processes
Advances in Photochemistry
Advances in physical Organic Chemistry
Advances in Protein Chemistry
Advances in Theoretically Interesting Molecules
Fluorine Chemistry Reviews
Fortschritte der Chemie Organischer Naturstoffe
Isotopes in Organic Chemistry
Molecular Structure and Energetics
Organic Photochemistry
Organometallic Reactions
Organic Reactions
Organic Synthesis: Theory and Applications
Progress in Heterocyclic Chemistry
Progress in Macrocyclic Chemistry
Progress in physical Organic Chemistry
Reactive Intermediates (Plenum)
Reactive Intermediates (Wiley)
Survey of Progress in Chemistry
Topics in physical Organometallic Chemistry
Topics in Stereochemistry

all review articles in the field of organic chemistry that have appeared in the preceding 3 months, including those in the review journals and serials mentioned above, as well as those in monographs and treatises. There is also a listing of new monographs on a single subject. Each list includes a subject index.

Another publication is the *Index of Reviews in Organic Chemistry*, compiled by Lewis, Chemical Society, London, a classified listing of review articles. The first volume, published in 1971, lists reviews from ~1960 (in some cases much earlier) to ≈ 1970 in alphabetical order of topic. Thus four reviews are listed under “Knoevenagel condensation,” five under “Inclusion compounds,” and one under “Vinyl ketones.” There is no index. A second volume (1977) covers the literature to 1976. Annual or biannual supplements appeared from 1979 until the publication was terminated in 1985. Classified lists of review articles on organometallic chemistry are found in articles by Smith and Walton³⁶ and by Bruce.³⁷ A similar list for heterocyclic chemistry is found in articles by Katritzky and others.³⁸ See also the discussion of the *Index of Scientific Reviews*, p. 1908.

Annual Reviews

The review articles discussed in the previous section are each devoted to a narrow topic covering the work done in that area over a period of years. An annual review is a publication that covers a broad area, but limits the period covered, usually to 1 or 2 years.

1. The oldest annual review publication still publishing is *Annual Reports on the Progress of Chemistry*, published by the Royal Society of Chemistry (formerly the chemical Society), which began in 1905 and which covers the whole field of chemistry. Since 1967 it has been divided into sections. Organic chemistry is found in Section B.
2. Because the number of papers in chemistry has become so large, the Royal Society of Chemistry publishes annual-review-type volumes of smaller scope, called *Specialist Periodical Reports*. Among those of interest to organic chemists are “Carbohydrate Chemistry” (Vol. 22 covers 1988); “Photochemistry” (Vol. 21 covers 1988–1989); and “General and Synthetic Methods,” (Vol. 12 covers 1987).
3. *Organic Reaction Mechanisms*, published by Wiley, New York, is an annual survey that covers the latest developments in the field of mechanisms. The first volume, covering 1965, appeared in 1966.
4. There are two annual reviews devoted to progress in organic synthesis. Theilheimer, *Synthetic Methods of Organic Chemistry*, S. Karger Verlag,

³⁶Smith, J.D.; Walton, D.R.M. *Adv. Organomet. Chem.* **1975**, *13*, 453.

³⁷Bruce, M.I.K. *Adv. Organomet. Chem.* **1972**, *10*, 273, **1973**, *11*, 447, **1974**, *12*, 380.

³⁸Belen'kii, L.I. *Adv. Heterocyclic Chem.* **1988**, *44*, 269; Katritzky, A.R.; Jones, P.M. *Adv. Heterocyclic Chem.* **1979**, *25*, 303; Katritzky, A.R.; Weeds, S.M. *Adv. Heterocyclic Chem.* **1966**, *7*, 225.

Basel, is an annual compilation, beginning in 1946, of new methods for the synthesis of organic compounds, arranged according to a system based on bond closing and bond breaking reactions. Equations, brief procedures, yields, and literature references are given. Volume 44 was issued in 1990. Volumes 3 and 4 are available only in German, but all the rest are in English. There is an index to each volume. Cumulative indexes appear in every fifth volume. Beginning with Vol. 8, each volume includes a short summary of trends in synthetic organic chemistry. A more recent series is *Annual Reports in Organic Synthesis*, Academic Press, New York, which has covered the literature of each year since 1970. Equations are listed with yields and references according to a fairly simple system.

5. The *Journal Of Organometallic Chemistry* several times a year publishes annual surveys arranged according to metallic element. For example, Vol. 404, published in February 1991, contains annual surveys for 1989 of organic compounds containing Sb, Bi, and Fe, and the use of transition metals in organic synthesis, and surveys for 1988 covering B, Ru, and Os.

Awareness Services

Besides the annual reviews and the title and abstract services previously mentioned, there exist a number of publications designed to keep readers aware of new developments in organic chemistry or in specific areas of it.

1. *Chemtracts: Organic Chemistry* is a bimonthly periodical, begun in 1988, that prints abstracts of certain recently published papers (those that the editors consider most important), with commentaries on these papers by distinguished organic chemists. Important current research in bioorganic, organometallic, synthesis, physical-organic and theoretical chemistry, and pharmaceutical–medicinal chemistry is covered in each issue, giving readers updates on the newest trends and developments in organic chemistry by summarizing and commenting on current and past research..
2. The Institute for Scientific Information (ISI), besides publishing *Current Contents* (p. 1877) and the *Science Citation Index* (p. 1877), also publishes *Index Chemicus* (formerly called *Current Abstracts of Chemistry and Index Chemicus*). This publication, begun in 1960 and appearing weekly, is devoted to printing structural formulas of all new compounds appearing in >100 journals, along with equations to show how they were synthesized and an author's summary of the work. Each issue contains five indexes: author, journal, biological activity, labeled compounds, and intermediates that were not isolated. These indexes are cumulated annually.
3. Theilheimer and the *Annual Reports on Organic Synthesis*, mentioned in the previous section, list new synthetic methods once a year. There are several publications that do this monthly. Among these are *Current Chemical Reactions* (begun in 1979 and published by ISI), *Journal of Synthetic*

Methods (begun in 1975 and published by Derwent publications), and *Methods in Organic Synthesis*, begun in 1984 and published by the Royal Society of Chemistry. *Methods in Organic Synthesis* also lists books and review articles pertaining to organic synthesis.

4. *Natural Product Updates*, a monthly publication begun in 1987 and published by the Royal Society of Chemistry, lists recent results in the chemistry of natural products, along with structural formulas. It covers new compounds, structure determinations, new properties and total syntheses, among other topics.

General Treatises

There are a number of large-scale multivolume treatises that cover the whole field of organic chemistry or large areas of it.

1. *Rodd's Chemistry of Carbon Compounds*, edited by Coffey, Elsevier, Amsterdam, The Netherlands, is a treatise consisting of five main volumes, each of which contains several parts. publication began in 1964 and is not yet complete. The organization is not greatly different from most textbooks, but the coverage is much broader and deeper. Supplements to many of the volumes have appeared. An earlier edition, called *Chemistry of Carbon Compounds*, edited by Rodd, was published in 10 parts from 1951 to 1962.
2. Houben–Weyl's, *Methoden der Organischen Chemie*, Georg Thieme Verlag, Stuttgart, is a major treatise in German devoted to laboratory methods. The fourth edition, which was begun in 1952 and consists of 20 volumes, most of them in several parts, is edited by E. Muller. The series includes supplementary volumes. The first four volumes contain general laboratory methods, analytical methods, physical methods, and general chemical methods. The later volumes are devoted to the synthesis of specific types of compounds, for example, hydrocarbons, oxygen compounds, and nitrogen compounds. Beginning in 1990 parts of the series have appeared in English.
3. *Comprehensive Organic Chemistry*, Pergamon, Elmsford, NY, 1979, is a six-volume treatise on the synthesis and reactions of organic compounds. The first three volumes cover the various functional groups, Vol. 4, heterocyclic compounds, and Vol. 5, biological compounds, such as proteins, carbohydrates, and lipids. Probably the most useful volume is Vol. 6, which contains formula, subject, and author indexes, as well as indexes of reactions and reagents. The last two of these not only refer to pages within the treatise, but directly give references to review articles and original papers. For example, on p. 1129, under "Chromic acid-sulphuric acid (Jones reagent), oxidation, alcohols," are listed 13 references to original papers. Several similar treatises, including the nine-volume *Comprehensive Organometallic Chemistry* (1982), the eight volume *Comprehensive Heterocyclic Chemistry* (1984), and the six volume *Comprehensive Medicinal Chemistry* (1989) are also published by Pergamon. The indexes to these works also include references.

4. A major treatise devoted to experimental methods of chemistry is *Techniques of Chemistry*, edited first by Weissberger and then by Saunders, Wiley, New York. This publication, which began in 1970, so far consists of 21 volumes, most of them in several parts, covering such topics as electrochemical and spectral methods, kinetic methods, photochromism, and organic solvents. *Techniques of Chemistry* is a successor to an earlier series, called *Techniques of Organic Chemistry*, which appeared in 14 volumes, some of them in more than one edition, from 1945 to 1969.
5. *Comprehensive Chemical Kinetics*, edited by Bamford and Tipper, 1969–, Elsevier, Amsterdam, The Netherlands, is a multivolume treatise covering the area of reaction kinetics. Six of these volumes (not all published at the time of writing) deal with the kinetics and mechanisms of organic reactions in a thorough and comprehensive manner.
6. Three multivolume treatises that cover specific areas are Elderfield, *Heterocyclic Compounds*, Wiley, New York, 1950–; Manske and Holmes, *The Alkaloids*, Academic Press, New York, 1950–; and Simonson, Owen, Barton, and Ross, *The Terpenes*, Cambridge University Press, London, 1947–1957.
7. *Encyclopedia of Reagents for Organic Synthesis*, edited by Paquette, Wiley, New York, was published in 1995. It is an eight volume, alphabetic listing of reagents used in organic chemistry with descriptions of the preparation, use and chemistry, with references. Each reagent was researched by organic chemists active in research, who contributed to the total publication.

This work is available on-line as **eEROS**. The *Encyclopedia of Reagents for Organic Synthesis*, e-EROS, provides updated information on ~3800 reagents with a database of close to 50,000 reactions. Each reagent entry includes properties such as physical data, solubility, form supplied in, purification, and preparative methods; examples of use in reactions; and literature references. Search options include: name, CAS number, structure and reaction.
8. *Comprehensive Organic Synthesis*, edited by Trost and Fleming, Pergamon, was published in 1991. It is a nine volume compilation.
9. *Comprehensive Organic Functional Group Transformations*, edited by Katritzky, Meth-Cohn, and Rees, Pergamon, was published in 1995. It is a seven volume compilation.

Monographs and Treatises on Specific Areas

Organic chemistry is blessed with a large number of books devoted to a thorough coverage of a specific area. Many of these are essentially very long review articles, differing from ordinary review articles only in size and scope. Some of the books are by a single author, and others have chapters by different authors but all are carefully planned to cover a specific area. Many of these books have been referred to in footnotes in appropriate places in this book. There have been several series of monographs, one of which is worth special mention: *The Chemistry of Functional Groups*, under the general editorship of Patai, published by

Wiley, New York. Each volume deals with the preparation, reactions, and physical and chemical properties of compounds containing a given functional group. Volumes covering >20 functional groups have appeared so far, including books on alkenes, cyano compounds, amines, carboxylic acids and esters, and quinones.

Textbooks

There are many excellent textbooks in the field of organic chemistry. We restrict ourselves to listing only a few of those published, mostly since 1985. Some of these are first-year texts and some are advanced (advanced texts generally give references; first-year texts do not, though they may give general bibliographies, suggestions for further reading, etc.); some cover the whole field, and others cover reactions, structure, and/or mechanism only. All the books listed here are not only good textbooks and the advanced books are valuable reference books for graduate students and practicing chemists.

Bruckner, *Advanced Organic Chemistry: Reaction Mechanisms*, Academic Press, NY **2001**.

Bruice, *Organic Chemistry*, 4th ed., Prentice-Hall, NJ, **2004**.

Carey, *Organic Chemistry*, 6th ed., McGraw-Hill, NY, **2006**.

Carey and Sundberg, *Advanced Organic Chemistry: Structure and Mechanisms (Part A)*, 4th ed., Springer, **2004**.

Carey and Sundberg, *Advanced Organic Chemistry: Structure and Mechanisms (Part B)*, 4th ed., Springer, **2001**.

Carruthers and Coldham, *Some Modern Methods of Organic Synthesis*, 4th ed., Cambridge University Press, Cambridge, **2004**.

Ege, *Organic Chemistry: Structure and Reactivity*, 5th ed., D.C. Houghton Mifflin, Boston, **2003**.

Fox and Whitesell, *Organic Chemistry*, 3rd ed, Jones and Bartlett, Sudbury, MA, **2004**.

Grossman, *The Art of Writing Reasonable Organic Reaction Mechanisms*, 2nd ed, Springer, **2005**.

House, *Modern Synthetic Reactions*, 2nd ed., W. A. Benjamin, New York, **1972**.

Ingold, *Structure and Mechanism in Organic Chemistry*, 2nd ed., Cornell University Press, Ithaca, NY, **1969**.

Isaacs, *Physical Organic Chemistry*, Wiley, NY, **1987**.

Jones, *Organic Chemistry*, 3rd ed. W.W. Norton, NY, **2004**.

Loudon, *Organic Chemistry*, 4th ed., Oxford University Press, Cambridge, **2001**.

Lowry and Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd ed., Harper and Row, New York, **1987**.

McMurry, *Organic Chemistry*, 6th ed., Brooks/Cole, Monterey CA, **2003**.

- Maskill, *The Physical Basis of Organic Chemistry*, Oxford University Press, Oxford, **1985**.
- Morrison, Boyd and Boyd, *Organic Chemistry*, 6th ed., Benjamin Cummings, CA, **1992**.
- Mundy, Ellerd, and Favalaro, Jr., *Name Reactions and Reagents in Organic Synthesis*, 2nd ed, Wiley, Hoboken, ND, **2005**.
- Ritchie, *Physical Organic Chemistry*, 2nd ed., Marcel Dekker, NY, **1989**.
- Solomons and Fryhle, *Organic Chemistry*, 8th ed., Wiley, NY, **2003**.
- Smith, *Organic Synthesis*, 2nd edition McGraw-Hill, NY, **2000**.
- Streitwieser, Heathcock, and Kosower, *Introductory Organic Chemistry*, 4th ed., Prentice-Hall, Saddle River, NJ, **1998**.
- Sykes, *A Guidebook to Mechanism in Organic Chemistry*, 6th ed., Longmans Scientific and Technical, Essex, **1986**.
- Vollhardt and Schore, *Organic Chemistry*, 4th ed., W.H. Freeman, New York, **2002**.
- Wade, *Organic Chemistry*, 4th ed., Prentice-Hall, Upper Saddle River, NJ, **1999**.

Other Books

In this section, we mention several books that do not fit conveniently into the previous categories. All but the last have to do with laboratory synthesis.

1. *Organic Syntheses*, published by Wiley, New York is a collection of procedures for the preparation of specific compounds. The thin annual volumes have appeared each year since 1921. For the first 59 volumes, the procedures for each 10- (or 9-) year period are collected in cumulative volumes. Beginning with Vol. 60, the cumulative volumes cover five-year periods. The cumulative volumes published so far are

Annual Volumes	Collective Volumes
1-9	I
10-19	II
20-29	III
30-39	IV
40-49	V
50-59	VI
60-64	VII
65-69	VIII
70-74	IX
75-80	X

The advantage of the procedures in *Organic Syntheses*, compared with those found in original journals, is that these procedures are *tested*. Each preparation is

carried out first by its author, and then by a member of the *Organic Syntheses* editorial board, and only if the yield is essentially duplicated is the procedure published. While it is possible to repeat most procedures given in journals, this is not always the case. All *Organic Syntheses* preparations are noted in *Beilstein* and in *CA*. In order to locate a given reaction in *Organic Syntheses*, the reader may use the OS references given in the present volume (through OS 69); the indexes in *Organic Syntheses* itself; Shriner and Shriner, *Organic Syntheses* Collective Volumes I, II, III, IV, V *Cumulative Indices*, Wiley, New York, 1976, or Sugasawa and Nakai; Reaction Index of *Organic Syntheses*, Wiley, New York, 1967 (through OS 45). Another book classifies virtually all the reactions in *Organic Syntheses* (collective vols. I–VII and annual vols. 65–68) into 11 categories: annulation, rearrangement, oxidation, reduction, addition, elimination, substitution, C–C bond formation, cleavage, protection–deprotection, and miscellaneous. This is *Organic Syntheses: Reaction Guide*, by Liotta and Volmer, published by Wiley, New York, in 1991. Some of the categories are subdivided further, and some reactions are listed in more than one category. What is given under each entry are the equation and the volume and page reference to *Organic Syntheses*.

2. Volume 1 of *Reagents for Organic Synthesis*, by Fieser and Fieser, Wiley, New York, 1967, is a 1457–page volume that discusses, in separate sections, some 1120 reagents and catalysts. It tells how each reagent is used in organic synthesis (with references) and, for each, tells which companies sell it, or how to prepare it, or both. The listing is alphabetical. Eighteen additional volumes have so far been published, which continue the format of Vol. 1 and add more recent material. A cumulative index for Vols. 1–12, by Smith and Fieser, was published in 1990. A complete cumulative index for Vol. 1–22 was published in 2005, by M.B. Smith. The series included Vol. 1–18 with Mary Fieser. After the death of Mary Fieser, the series was resumed by T. -L. Ho, and now includes Vol. 19–22.
3. *Comprehensive Organic Transformations*, 2nd ed. by Larock, Wiley-VCH, New York, 1999, has been frequently referred to in footnotes in Part 2 of this book. This compendium is devoted to listings of methods for the conversion of one functional group into another, and covers the literature through 1987. It is divided into nine sections covering the preparation of alkanes and arenes, alkenes, alkynes, halides, amines, ethers, alcohols and phenols, aldehydes and ketones, and nitriles, carboxylic acids and derivatives. Within each section are given many methods for synthesizing the given type of compound, arranged in a logical system. A schematic equation is given for each method, and then a list of references (without author names, to save space) for locating examples of the use of that method. When different reagents are used for the same functional group transformation, the particular reagent is shown for each reference. There is a 164–page index of group transformations. The 2nd edition has only recently been published and is *not* referenced in this edition, and a CD ROM version is now available.

4. *Survey of Organic Synthesis*, by Buehler and Pearson, Wiley, New York, 2 vols., **1970, 1977**, discusses hundreds of reactions used to prepare the principal types of organic compounds. The arrangement is by chapters, each covering a functional group, (e.g., ketones, acyl halides, amines). Each reaction is thoroughly discussed and brief synthetic procedures are given. There are many references.
5. A similar publication is Sandler and Karo, *Organic Functional Group Preparations*, 2nd ed., 3 vols., Academic Press, New York, **1983–1989**. This publication covers more functional groups than Buehler and Pearson.
6. *Compendium of Organic Synthetic Methods*, Wiley, New York, contains equations describing the preparation of thousands of monofunctional and difunctional compounds with references. Eleven volumes have been published so far (vol. 1–2, edited by Harrison and Harrison; Vol. 3, edited by Hegedus and Wade; Vol. 4–5, edited by Wade; Vol. 6–11 edited by Smith). Volume 12 will appear in 2007.
7. *The Vocabulary of Organic Chemistry*, by Orchin, Kaplan, Macomber, Wilson, and Zimmer, Wiley, New York, **1980**, presents definitions of >1000 terms used in many branches of organic chemistry, including stereochemistry, thermodynamics, wave mechanics, natural products, and fossil fuels. There are also lists of classes of organic compounds, types of mechanism, and name reactions (with mechanisms). The arrangement is topical rather than alphabetical, but there is a good index. *Compendium of Chemical Terminology*, by Gold, Loening, McNaught, and Sehmi (the “Gold book”), published by Blackwell Scientific publications, Oxford, in 1987, is an official IUPAC list of definitions of terms in several areas of chemistry, including organic.

LITERATURE SEARCHING

Until recently searching the chemical literature meant looking only at printed materials (some of which might be on microfilm or microfiche). Now, however, much of the literature can be searched online, including some of the most important. Whether the search is online or uses only the printed material, there are two basic types of search, (1) searches for information about one or more specific compounds or classes of compounds, and (2) other types of searches. First, we will discuss searches using only printed materials, and then on-line searching.³⁹

Literature Searching Using Printed Materials

Searching for Specific Compounds. Organic chemists often need to know if a compound has ever been prepared and if so, how, and/or they may be seeking a melting point, an ir spectrum, or some other property. Someone who wants all

³⁹For a monograph that covers both online searching and searching using printed materials, see Wiggins, *G. Chemical Information Sources*, McGraw-Hill: NY, **1991**.

the information that has ever been published on any compound begins by consulting the formula indexes in *Beilstein* (p. 1883). At this time there are two ways to do this. (1) The formula index to the second supplement (Vol. 29, see p. \$\$\$) will quickly show whether the compound is mentioned in the literature through 1929. If it is there, the searcher turns to the pages indicated, where all methods used to prepare the compound are given, as well as all physical properties, with references. Use of the page heading method described on p. 1882 will then show the locations, if any, in the third and later supplements. (2) If one has an idea which volume of *Beilstein* the compound is in (and the tables of contents at the front of the volumes may help), one may search the cumulative index for that volume. If not sure, one may consult several indexes. One of these two procedures will locate all compounds mentioned in the literature through 1959. If the compound is heterocyclic, it may be in the fifth supplement. If it is in Vols. 17–19 (or in a later volume whose index has been published), the corresponding indexes may be consulted. If not, the page heading method will find it, if it was reported before 1960.⁴⁰ There is a way by which all of the above can be avoided. A computer program, called SANDRA (available from the *Beilstein* publisher), allows the user to find the *Beilstein* location by using a mouse to draw the structural formula of the compound sought. At this point, the investigator will know (1) all information published through 1959 or 1979,³⁴ or (2) that the compound is not mentioned in the literature through 1959 or 1979.⁴¹ In some cases, scrutiny of *Beilstein* will be sufficient, perhaps if only a boiling point or a refractive index is required. In other cases, especially where specific laboratory directions are needed, the investigator will have to turn to the original papers.

To carry the search past 1959 (or 1979), the chemist next turns to the collective formula indexes of *Chemical Abstracts*TM: 1957–1961; 1962–1966; 1967–1971; 1972–1976; 1977–1981; 1982–1986; 1987–1991; 1992–1996; 1997–2002, and such later collective indexes as have appeared; and the semiannual indexes thereafter. If a given formula index contains only a few references to the compound in question, the pages or abstract numbers will be given directly in the formula index. However, if there are many references, the reader will be directed to see the chemical substance index or (before 1972) the subject index for the same period; and here the number of page or abstract numbers may be very large indeed. Fortunately, numerous subheadings are given, and these often help the user to narrow the search to the more promising entries. Nevertheless, one will undoubtedly turn to many abstracts that do not prove to be helpful. In many cases, the information in the abstracts will be sufficient. If not, the original references must be consulted. In some cases (the index entry is marked by an asterisk or a double asterisk), the

⁴⁰Compounds newly reported in the fifth supplement that are in a volume whose index has not yet been published will not be found by this procedure. To find them in *Beilstein* it is necessary to know something about the system (see Ref. 25), but they may also be found by consulting *CA* indexes beginning with the sixth collective index, or by using *Beilstein* on-line.

⁴¹For those heterocyclic compounds that would naturally belong to a volume for which the fifth supplement has been published.

compound is not mentioned in the abstract, though it is in the original paper or patent. Incidentally, all entries in the *CA* indexes that refer to patents are prefixed by the letter P. Since 1967, the prefixes B and R have also been used, to signify books and reviews, respectively.

By the procedure outlined above, all information regarding a specific compound that has been published up to about 1 year before the search can be found by a procedure that is always straightforward and that in many cases is rapid (if the compound has been reported only a few times). Equally important, if the compound has not been reported, the investigator will know that, too. It should be pointed out that for common compounds, such as benzene, ether, acetone, trivial mentions in the literature are not indexed (so they will not be found by this procedure), only significant ones. Thus, if acetone is converted to another compound, an index entry will be found, but not if it is used as a solvent or an eluant in a common procedure.

The best way to learn if a compound is mentioned in the literature after the period covered by the latest semiannual formula index of *CA* is to use the online services. However, if one lacks access to these, one may consult the keyword index at the end of each issue of *CA*. In these cases, of course, it is necessary to know what name might be used for the compound. The name is not necessary for *Index Chemicus*; one consults the formula indexes. However, these methods are far from complete. *Index Chemicus* lists primarily new compounds, those that would not have been found in the earlier search. The keyword indexes in *CA* are more complete, being based on internal subject matter, as well as title, but they are by no means exhaustive. Furthermore, all three of these publications lag some distance behind the original journals. To locate all references to a compound after the period covered by the latest semiannual formula index of *CA*, it is necessary to use *CAS* on-line.

The complete procedure described above may not be necessary in all cases. Often all the information one needs about a compound will be found in one of the handbooks (p. 1887), in the *Dictionary of Organic Compounds* (p. 1885), or in one of the other compendia listed in this chapter, most of which give references to the original literature.

Other Searches.⁴² There is no definite procedure for making other literature searches using only printed materials. Any chemist who wishes to learn all that is known about the mechanism of the reaction between aldehydes and HCN, or which compounds of the general formula Ar_3CR have been prepared, or which are the best catalysts for Friedel–Crafts acylation of naphthalene derivatives with anhydrides, or where the group $-\text{C}(\text{NH}_2)=\text{N}-$ absorbs in the IR, is dependent on their ingenuity and knowledge of the literature. If a specific piece of information is needed, it may be possible to find it in one of the compendia mentioned previously. If the topic is more general, the best procedure is often to begin by consulting one or more monographs, treatises, or textbooks that will give general

⁴²This discussion is necessarily short. For much more extensive discussions, consult the books in Refs. 1 and 17.

background information and often provide references to review articles and original papers. In many cases, this is sufficient, but when a complete search is required, it is necessary to consult the *CA* subject and/or chemical substance indexes, where the ingenuity of the investigator is most required, for now it must be decided which words to look under. If one is interested in the mechanism of the reaction between aldehydes and HCN, one might look under “aldehydes,” or “hydrogen cyanide,” or even under “acetaldehyde” or “benzaldehyde,” and so on, but then the search is likely to prove long. A better choice in this case would be “cyanohydrin,” since these are the normal products and references there would be fewer. It would be a waste of time to look under “mechanism.” In any case, many of the abstracts would not prove helpful. Literature searching of this kind is necessarily a wasteful process. Of course, the searcher would not consult the *CA* annual indexes, but only the collective indexes as far as they go and the semiannual indexes thereafter. If it is necessary to search before 1907 (and even before 1920, since *CA* was not very complete from 1907 to ~1920), recourse may be made to *Chemisches Zentralblatt* and the abstracts in the *Journal of the Chemical Society*.

Literature Searching Online³⁹

Most of the *Chemical Abstracts*TM literature can be accessed using CAS databases on-line. The CAS registry⁴³ is the largest and most current database of chemical substance information in the world containing >26 million organic and inorganic substances and 56 million sequences. CAS is a team of scientists who provide digital information environment for scientific research and discovery and provides pathways to published research in the world's journal and patent literature back to the beginning of the twentieth century. Since 1907, CAS has indexed and summarized chemistry-related articles from >40,000 scientific journals, in addition to patents, conference proceedings and other documents pertinent to chemistry, life sciences and many other fields. In total, abstracts for >24 million documents are accessible online through CAS. Through the printed *CA*, *CA* on CD, STN, the CAS files distributed through licensed vendors, the SciFinder[®] and SciFinder ScholarTM desktop research tools, and the STN[®] Easy or STN[®] on the Web services, data produced by CAS is accessible to virtually any scientific researcher worldwide in industry, governmental research institutions, and academia.

Substance identification is a special strength of CAS. It is widely known as the CAS Registry, the largest substance identification system in existence. When a chemical substance, newly encountered in the literature, is processed by CAS, its molecular structure diagram, systematic chemical name, molecular formula, and other identifying information are added to the Registry and it is assigned a unique CAS Registry Number[®]. Registry now contains records for >26 million organic and inorganic substances and >56 million sequences.

The CAS REGISTRY contains >27 million organic and inorganic substances and >57 million sequences. A current count of substance records like this is

⁴³<http://www.cas.org/about.html>

updated daily on the CAS web site.⁴⁴ An important piece of information that assists in such a search is the CAS Registry Number[®]. Each substance in REGISTRY is identified by a unique numeric identifier called a CAS Registry Number[®].⁴⁵ “The CAS Registry Number[®] is a unique number assigned to a chemical by the Chemical Abstracts Service.⁴⁶ A fairly large collection of CAS numbers, with links to safety data for many chemicals, can be found at the listing of chemicals by CAS number at the Safety Home Page of the Physical and Theoretical Chemistry Laboratory at Oxford University.”⁴⁷ The CAS Registry Number[®] is a unique numeric identifier that designates only one substance, has no chemical significance, and is a link to finding information about a specific chemical substance. A CAS Registry Number[®] includes up to nine digits that are separated into three groups by hyphens. The first part of the number, starting from the left, has up to six digits; the second part has two digits. The final part consists of a single check digit.⁴⁸

CAS is located in Columbus, Ohio and is a division of the American Chemical Society. CAS can be contacted at Chemical Abstracts Service, 2540 Olentangy River Road, P.O. Box 3012, Columbus, Ohio 43210 (E-mail: help@cas.org).

Online searching means using a computer terminal to search a *database*. Although databases in chemistry are available from several organizations, STN[®] International (The Scientific & Technical Information Network) is important because it is comprehensive and available in many countries. STN[®] has dozens of databases, including many that cover chemistry and chemical engineering. To access these databases a chemistry department, a library, or an individual subscribes to STN[®] (for a nominal fee), and receives code numbers that will permit access to the system. Then all one needs is a computer and a modem. STN[®] charges for each use, depending on which databases are used, for how long, and what kind of information is requested. One of the nice features of STN[®] is that the same command language is used for all databases, so when one has mastered the language for one database, one can use it for all the others. In this section, we will discuss literature searching using CAS databases online, which is one of the databases available from STN. One thing that must be remembered is that *CAS databases online* is complete only from 1967 to the present,⁴⁹ so that searches for earlier abstracts must use the printed volumes. However, for the period since 1967, not only is online searching a great deal faster than searching the printed CA, but, as we will see, one can do kinds of searches online that are simply not possible using only the printed volumes. Furthermore, the on-line files are updated every two weeks, so that one will find all the abstracts on-line well past the appearance of the latest semiannual indexes, often even before the library has received the latest

⁴⁴<http://www.cas.org/cgi-bin/regreport.pl>

⁴⁵<http://www.cas.org/EO/regsys.html>

⁴⁶<http://www.cas.org/>

⁴⁷<http://ptcl.chem.ox.ac.uk/MSDS/glossary/casnumber.html>

⁴⁸<http://www.cas.org/EO/checkdig.html>

⁴⁹There is also a file called CAOLD that has some papers earlier than 1967.

weekly printed issue of *CA*. The *CAS databases online* is extremely flexible; one can search in a great many ways. It is beyond the scope of this book to discuss the system in detail (*CA* conducts workshops on its use), but even with the few commands we will give here, a user can often find all that he or she is looking for. The *CAS databases online* has two major files, the *CA File* and the *Registry File*.⁵⁰ T

SciFinder[®]: A Search Tool for Exploring CAS Databases⁵¹

Tutorials are available to help use SciFinder[®],⁵² which is a searching tool and not the CAS database. SciFinder[®] can search a research topic⁵³ or a compound can be searched by structure.⁵⁴ Another search engine is available, different from SciFinder[®], known as STN Express[®] with Discover!,⁵⁵ and this searching tool can also be used to search CAS databases.⁵⁶ The Analysis Edition of STN Express[®] with Discover! allows one to search, analyze, visualize, and discover sci-tech information by the ability to create a table for substance analysis that identifies the common substructure for an answer set of structurally related substances; Group related author-inventor names and company names for better analysis and visualization results; Analyze and tabulate data from single- or multi-file search results, and create a data table and 3D chart; Save an answer set from databases such as CPlusSM, PCTFULL, and USPATFULL with the Save for STN[®] AnaVist Wizard, and then import and open it in STN[®] AnaVistTM; Create an interactive spreadsheet from all or only hit CAS Registry Number[®]s and their corresponding CAS Roles through the CAS Registry Number[®]; Upload lengthy genetic sequences automatically for searching in DGENE and PCTGEN via the Upload Query Wizard. STN Express[®] was developed in collaboration with Hampden Data Services. Note that the CPlus database makes it possible to see not only what a paper has cited, but also what papers it been cited by.

To illustrate how STN[®] is used, an on-line tutorial is available.⁵⁷ A few on-line windows from a SciFinder[®] search are provided to illustrate how searches can be done. This presentation is by no means complete or intended as an alternative to the actual tutorial. Indeed, one could *not* use SciFinder[®] properly after simply reading this discussion. The intent is to illustrate some features that are available and to present an overview of the use of this important tool.

⁵⁰There is also a file, LCA, which is used for learning the system. It includes only a small fraction of the papers in the CA File, and is not updated. There is no charge for using the LCA File, except for a small hourly fee.

⁵¹<http://www.cas.org/>. For a tutorial, see <http://www.cas.org/SCIFINDER/citation.html>.

⁵²<http://www.cas.org/SCIFINDER/SCHOLAR/interact/>

⁵³<http://www.cas.org/SCIFINDER/SCHOLAR/page2a.html>

⁵⁴<http://www.cas.org/SCIFINDER/SCHOLAR/scholstruc.html>

⁵⁵<http://www.cas.org/ONLINE/STN/discover.html>

⁵⁶<http://www.cas.org/stn.html>

⁵⁷<http://www.cas.org/ONLINE/STN/expressmac.pdf>

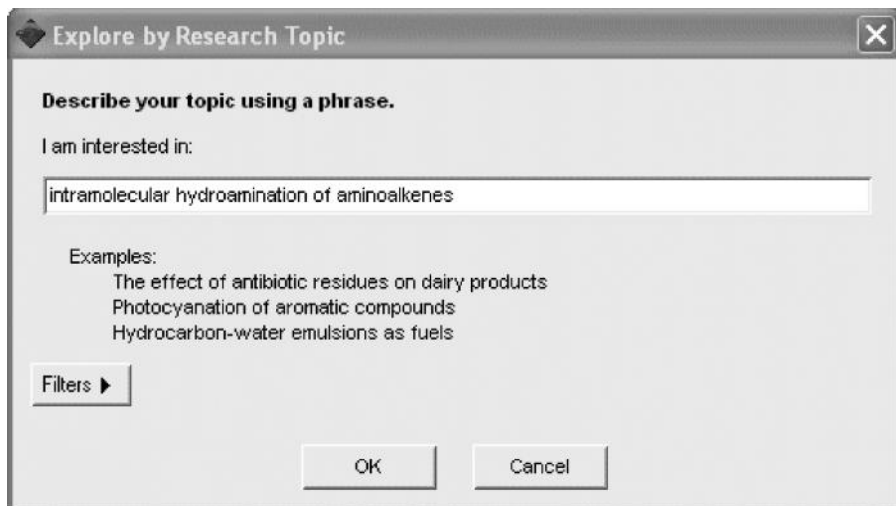


Fig. A.3. Explore by research topic.

Using SciFinder[®], a search can be done in one of several different ways. In one example, a search is done by research topic.⁵⁸ The example shown in Fig. A.3 shows a search for intramolecular hydroamination of aminoalkenes. To begin, click Explore by research topic and enter the appropriate information.

It is possible to use filters (see Fig. A.3) in order to refine the search by year, document type (journal, patent, review, etc.), author, or company. A window is returned containing references categorized by their relationship to the search phrase, as shown in Fig. A.4. One then simply checks those reference lists that appear closest to the area of interest.

After clicking on “get references,” a screen is returned (Fig. A.5) that has the original references as shown in the window. One is given the option of refining this list further, and for each reference, most browsers allow viewing of the abstract or the full references as an HTML or a pdf file. Two icons appear beside each reference in the list: a microscope, which can be clicked on to see the abstract, and an document icon that can be clicked on to see the full-text, original article on the publisher’s web-site. This feature is an alternative to document delivery in the traditional sense.

Other examples of typical searches allowed by SciFinder[®] include search by authors name, as with Professor K. Barry Sharpless shown in Fig. A.6. Search by structure is also possible, such as the one shown in Fig. A.7, and the program provides drawing tools. SciFinder[®] then searches to finds matches based on structure or reaction.

It is also possible to using the drawing tools to search by reaction and reaction type. SciFinder[®] returns reaction information, such as that shown in Fig. A. 8. In

⁵⁸<http://www.cas.org/SCIFINDER/topic.html>

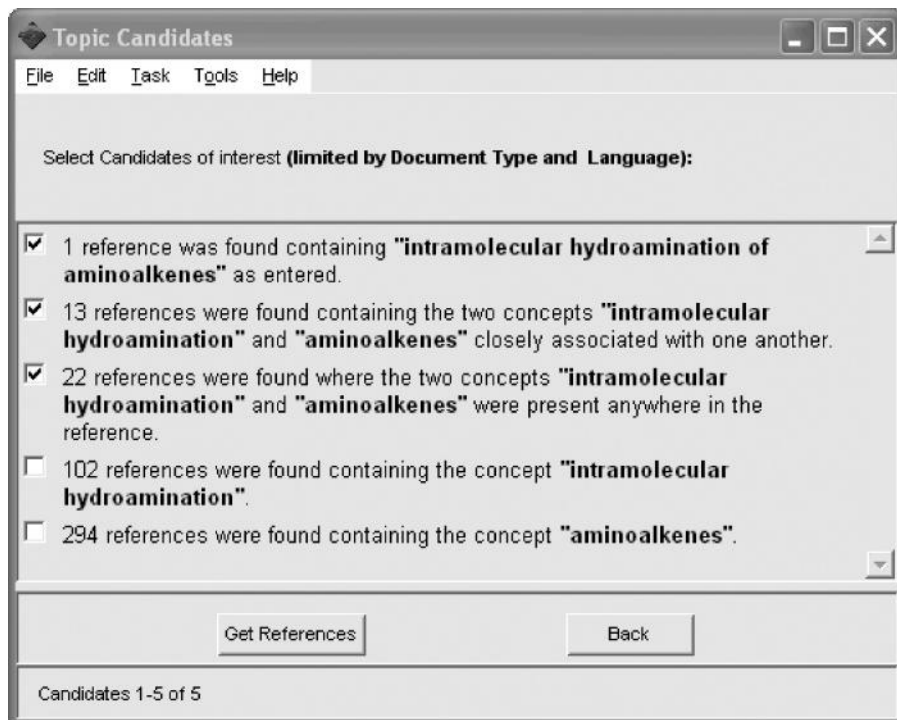


Fig. A.4. Selection of candidates of interest for search by research topic.

all cases, journal articles and/or patents are returned that provide direct access to the literature of interest.

Science Citation Index

As seen in the SciFinder[®] search tutorials, it is possible to track papers that have cited a particular article or author. A publication that can greatly facilitate literature searching is *Science Citation Index (SCI)*, begun in 1961. This publication, which is quite different from any other mentioned in this chapter, gives a list of all papers in a given year that have cited a given paper, patent, or book. Its utility lies in the fact that it enables the user to search *forward* from a given paper or patent, rather than backward, as is usually the case. For example, suppose a chemist is familiar with a paper by Jencks and Gilchrist (*J. Am. Chem. Soc.*, **1968**, *90*, 2622) entitled "Nonlinear Structure–Reactivity Correlations. The Reactivity of Nucleophilic Reagents toward Esters." The chemist is easily able to begin a search for earlier papers by using references supplied in this paper, and can then go further backward with the aid of references in those papers, and so on. But for obvious reasons, the paper itself supplies no way to locate *later* papers.

SciFinder

File Edit View Task Tools Help

NewTask Back Forward Print Save As FullText Prefs Database History Contact Internet Panorama Help Exit

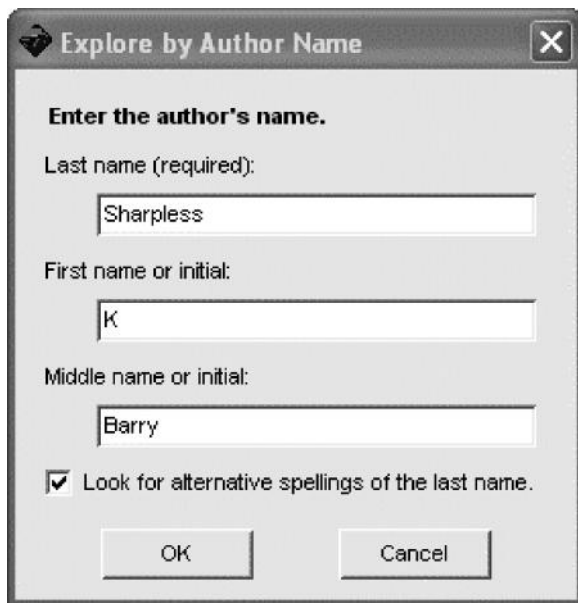
- Kim, Joon Young; Livinghouse, Tom. **Enantioselective Intramolecular Alkene Hydroaminations Catalyzed by Yttrium Complexes of Axially Chiral Bis(thiolate) Ligands.** *Organic Letters* (2005), 7(9), 1737-1739. CODEN: ORLEF7 ISSN:1523-7060. CAN 143:7568 AN 2005:289566 CAPLUS
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Fig. A.5. Original literature references returned for search by research topic.

The *SCI* is designed to make up for this gap. The citation index of *SCI* lists all papers, patents, or books cited in a given year or 2-month period (by first author only) and then gives a list of papers that have done the citing. The index is published bimonthly and cumulated annually. For example, column 43,901 of the 1989 citation index shows that the Jencks paper mentioned above was cited as a footnote in 16 papers published in 1989. It is reasonable to assume that most of the papers that cited the Jencks paper were on closely related subjects. For each of the 16 papers are listed the first author, journal abbreviation, volume and page numbers, and year. In a similar manner, if one consulted *SCI* for all the years from 1968 on, one would have a complete list of papers that cited that paper. One could obviously broaden the search by then consulting *SCI* (from 1989 on) for papers that cited these 16 papers, and so on. Papers, patents, or books listed, for example, in the 1989 *SCI* may go back many years (e.g., papers published by Einstein in 1905 and 1906 are included). The only



The screenshot shows a dialog box titled "Explore by Author Name" with a close button (X) in the top right corner. The dialog contains the following fields and options:

- Enter the author's name.**
- Last name (required):
- First name or initial:
- Middle name or initial:
- Look for alternative spellings of the last name.
- Buttons: OK and Cancel

Fig. A.6. Screen shot for beginning a search by author.

requirement is that a paper published in 1989 (or late 1988) has mentioned the earlier paper in a footnote. The arrangement of cited papers or books is alphabetical by cited first author and then by cited year. Cited patents are listed in a separate table, in order of patent number, though the inventor and country are also given.

The *SCI* covers ~3200 journals in the physical and biological sciences, as well as in medicine, agriculture, and technology. In addition to the citation index, each bimonthly and annual *SCI* also includes three other indexes. One of these, called *Source Index*, is similar to the *CA* author index. It lists the titles, journal abbreviations, volume, issue, page numbers, and year of all papers published by a given author during that 2-month period or year. All authors are listed; not just first authors. The second, called the *Corporate Index*, lists all publications that have been published from a given institution during that period, by first author. Thus, the corporate index for 1989 lists 63 papers by 45 different first authors emanating from the Department of Chemistry of Rutgers University, New Brunswick, NJ. The main section of the corporate index (the Geographic Section) lists institutions by country or (for the U.S.) by state. There is also an Organization Section, which lists the names of institutions alphabetically, and for each gives the location, so it can be found in the geographic section. The third index included in *SCI* is the *Permuterm*⁵⁹ *Subject Index*. This index alphabetically lists every significant word in the titles of

⁵⁹Registered trade name.

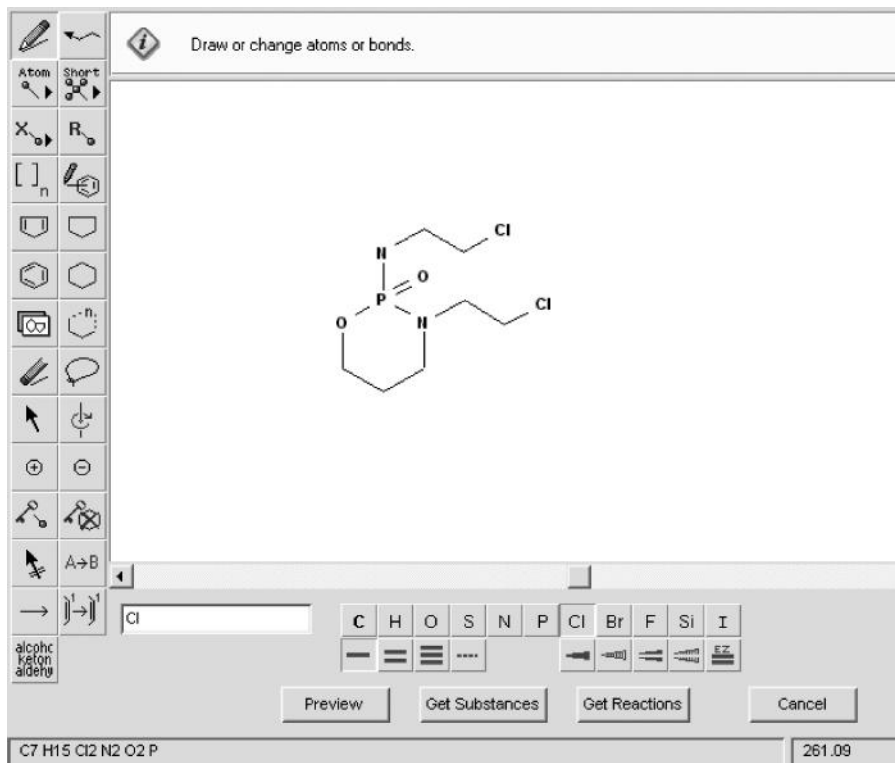


Fig. A.7. Screen shot for beginning a search by structure, using the drawing tools.

all papers published in that year or bimonthly period, paired with all other significant words in the same title. Thus, for example, a title with seven significant words appears at 42 separate places in the index. Each of the seven words appears six times as the main word, each time paired with a different word as the coword. The user is then led to the *Source Index*, where the full reference is given. The *SCI* is also available on-line (though not through STN) and on CD ROM disks. A version of *SCI* that is restricted to chemistry, but also includes searchable abstracts, is available only in the CD ROM format.

The publishers of *SCI* also produce another publication, called *Index to Scientific Reviews*, that appears semiannually. This publication, which began in 1974, is very similar to *SCI*, but confines itself to listing citations to review articles. The citations come from ~2500 journals in the same general areas as are covered by *SCI*. The review articles cited appeared in ~215 review journals and books, as well as in those journals that publish occasional review articles. Like *SCI*, the *Index to Scientific Reviews* contains citation, source, corporate, and Permuterm indexes. It also contains a "Research Front Specialty Index," which classifies reviews by subject.

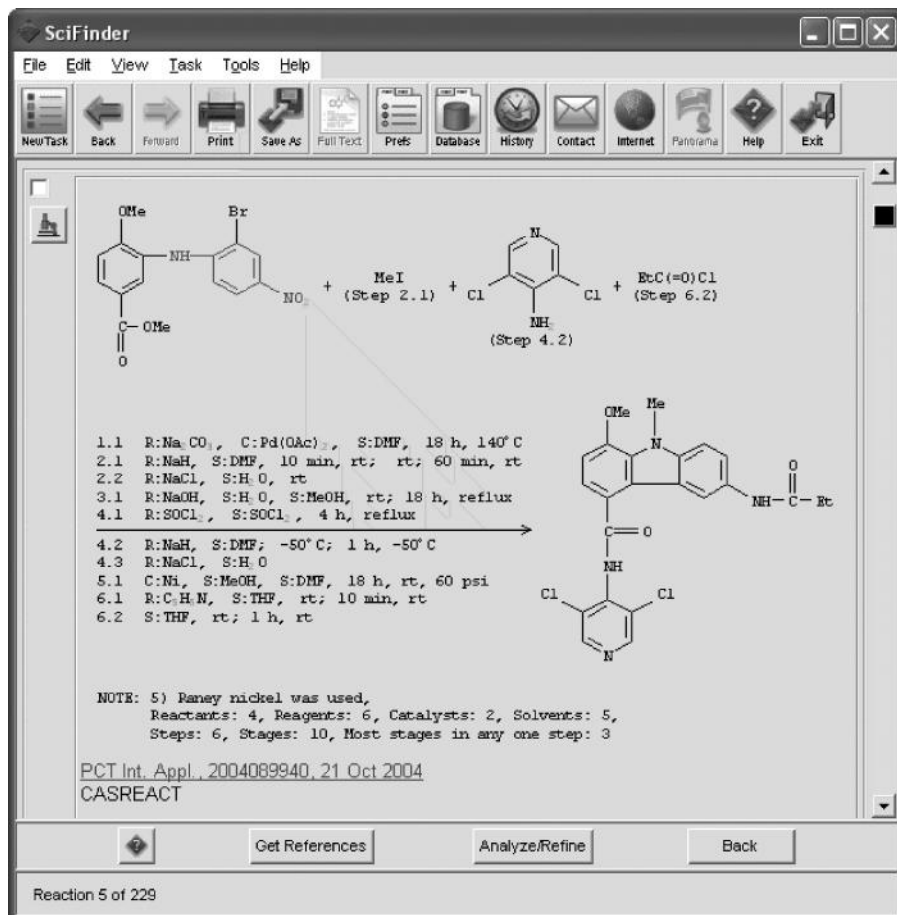


Fig. A.8. Screen shot of results for a search by reaction, using the drawing tools.

How to Locate Journal Articles

Having obtained a reference from various sources or searches, one often needs to consult the original journal (the location of patents is discussed on p. \$\$\$). The first step is to ascertain the full name of the journal, since it is the abbreviation that is generally given. Of course, everyone should be familiar with the abbreviations of the very important journals, such as *J. Org. Chem.*, *Angew. Chem. Int. Ed.*, and so on, but references are often found to journals whose titles are not at all familiar (e.g., *K. Skogs Lantbruksakad. Tidskr.* or *Nauchn. Tr. Mosk. Lesotekh. Inst.*). In such cases, one consults the *Chemical Abstracts Service Source Index (CASSI)*, with the most recent abbreviations in bold print. *CASSI* is available in a 1907–2004 cumulative, containing information 80,000 serial and nonserial publications. *CASSI* also lists journals covered by *Chemisches Zentralblatt* and its predecessors

from 1830 to 1969, and journals cited in *Beilstein* before 1907. The journals are listed in alphabetical order of the *abbreviations*, not of the titles. Journal title changes have not been infrequent, and *CASSI* also contains all former names, with cross-references to the current names. Quarterly supplements, cumulated annually, to *CASSI* have appeared since 1990 listing new journals and recent changes in journal titles. It should be pointed out that, while many publications use the *CA* abbreviations, not all do. The student will find that usage will vary from country to country, and even from journal to journal within a country. Furthermore, the *CA* abbreviations have changed from time to time. Articles can be accessed directly from SciFinder[®] using the CAS ChemPort feature.⁶⁰

Once the complete title is known, the journal can easily be obtained if it is in the library customarily used by the chemist. If not, one must use another library, and the next step is to find out which libraries carry the journal. *CASSI* answers this question too, since it carries a list of some 360 libraries in the United States and other countries, and *for each journal it tells which of these libraries carries it*, and furthermore, if the holdings are incomplete, which volumes of that journal are carried by each library. It may be possible to visit the closest library personally. If not, a copy of the article can usually be obtained through interlibrary loan. *CASSI* also includes lists of journal publishers, sales agents, and document depositories. Photocopies of most documents cited in *CA* can be obtained from *Chemical Abstracts*[™] Document Delivery Service, Customer Services, 2540 Olentangy River Road, Columbus OH, 43210, U.S. Orders for documents can be placed by mail, telephone, Telex, fax, or on-line through STN[®] or other services.

These latter comments are largely out of date given the on-line status of most journals. As mentioned above, pdf files of an article can be downloaded, or they can be read directly via the HTML file using any current browser. The reader is encouraged to contact the library person in your establishment that is responsible for chemical literature and to learn which on-line services are available through your local library.

⁶⁰See <http://www.cas.org/chemport/index.html>

Classification of Reactions by Type of Compounds Synthesized

ACETALS		boranes + CO–oxidation	18-23
acetals + RM	10-64	boranes + CO–reduction	18-24
aldehydes + alcohols	16-05	by the Cannizzaro reaction	19-81
by transesterification	10-13	by Wittig rearrangement	18-21
from dihalides	10-8	cleavage of ethers	10-49
from hydroxy-ethers	14-06	condensation of aldehydes	19-81
ortho esters + RM	10-64	conjugate reduction	15-14
reductive cleavage of ortho esters	19-56	carboxylic esters + organometallics	16-82
		epoxides + organometallics	10-65
ACYLALS (DIESTERS)		epoxides + silanes	10-55
aldehydes + anhydrides	16-06	from boranes	10-01
		from boronates	18-23
ACYLOINS – see hydroxy ketones		Grignard addition to aldehydes or ketones	16-24
ALCOHOLS		hydration of alkenes	15-03
addition of other organometallics to carbonyls	16-25	hydrolysis of acetals and ketals	10-06
aldehydes + allylic silanes	16-51	hydrolysis of alkyl halides	10-01
alkenes + alcohols	15-33	hydrolysis of inorganic esters	10-04
alkenes + aldehydes or ketones	16-54	hydrolysis of sulfonate esters	10-04
alkenes-oxymercuration	15-03	hydrolysis of vinyl ethers	10-06
amides + organometallic compounds	16-82	hydroxylation at aliphatic carbon	19-14
amines + KOH	10-23	hydroxymethylation of arenes	11-12
anhydrides + organometallic compounds	16-82	organolithium addition to aldehydes or ketones	16-24
arylation of ketones	11-12	oxidation of boranes	12-27
		oxidation of boranes	15-16
		oxidation of methylene	19-15

oxidation of silanes	10-16	boranes + MeO(ArS)CH ₂ Li	18-24
radical addition to carbonyl compounds	16-56	by decarboxylation	12-40
		by Michael addition	15-24
rearrangement of ethers	18-22	by rearrangement of aldehydes	18-04
rearrangement of peroxides	18-20	by the Wacker process	19-25
reduction of acyl halides	19-63	carbonylation of aromatic compounds	11-18
reduction of aldehydes or ketones	19-36	carbonylation of hydrocarbons	12-33
reduction of carbonyls with Grignard reagents	16-24	formylation of aromatic compounds	11-18
reduction of carboxylic acids	19-37	from aryl imines	11-18
reduction of carboxylic esters	19-38	from dihydrooxazines	10-72
reduction of carboxylic esters	19-65	from dithioaldehydes	16-11
reduction of epoxides	19-35	hydroformylation	15-37
reduction peroxides	19-60	hydrolysis of acetals	10-06
ring expansion of amines	18-03	hydrolysis of C=N compounds	16-02
silanes + aldehydes or ketones	16-26	hydrolysis of <i>gem</i> -dihalides	10-02
		hydrolysis of nitro compounds	16-03
ALCOHOLS, ALLYLIC		hydrolysis of vinyl ethers	10-06
addition of allylic organometallics to carbonyls	16-25	oxidation of alcohols	19-03
alkenes + formaldehyde	16-54	oxidation of aryl methyl groups	19-18
allylic silanes + aldehydes or ketones	16-26	oxidation of nitro compounds	19-21
		oxidation of primary alkyl halides	19-20
deprotonation of epoxides	17-03	oxidative cleavage of diols	19-07
rearrangement of alkene-sulfoxides	18-35	oxidative cleavage of epoxides	19-07
		ozonolysis of alkenes	19-09
ALDEHYDES		reduction anhydrides	19-40
alkenes + aldehydes	15-33	reduction nitriles	19-44
alkyl halides + organoiron compounds	10-76	reduction of acyl halides	19-39
alkylation of aldehydes	10-68	reduction of acyl halides	19-40
alkylation of imines	10-68	reduction of amides	19-41
alkylation reactions and keto-enol tautomerism	10-67	reduction of carboxylic acids	19-40
	12-03	reduction of carboxylic esters	19-40
aromatic compounds + chloroform	11-18	ALKANES	
aromatic compounds + formaldehyde	11-18	addition of alkanes to alkenes	15-18
aromatic compounds + formamides	11-18	alcohols + RM	10-63
aromatic compounds + halo-ethers	11-18	alkenes + diimide	15-12
arylation of aldehydes	13-14	alkenes + metals	15-12
		alkenes + organometallics	15-21
		alkyl halides + metals	10-56
		alkyl halides + metals	10-56
		alkyl halides + organocuprates	10-58
		alkyl halides + RM (Li, Na, K)	10-57

alkyl halides + RM (other metals)	10-59	replacement of metals in RM by hydrogen	12-24
alkyl halides + silanes	10-55	σ -bond rearrangements	18-38
Barton–McCombie reaction	19-58	sulfonate esters + metals	10-56
by decarboxylation	12-40	sulfonate esters + organocuprates	10-58
by [3+2]-cycloaddition	15-59	sulfonyl compounds + organometallics	10-61
cleavage of alkanes	12-47	via transmetallation	12-22
cleavage of ketones	12-46		
coupling of boranes	14-26	ALKENE-ALCOHOLS	
coupling of carboxylate salts	14-29	rearrangement of alkene-ethers	18-35
coupling of Grignard reagents	14-24		
coupling of organocuprates	14-25	ALKENE-ALDEHYDES	
coupling of two alkanes	14-15	Claisen rearrangement	18-33
decarbonylation of aldehydes	14-32	Cope rearrangement	18-32
decyanation	12-48	rearrangement of allyl vinyl ethers	18-33
from alcohols	19-58		
from alkylborates	10-59	ALKENE-ALKYNES	
from boranes	10-59	addition of alkynes to alkynes	15-20
hydrogen exchange	12-01		
hydrogenation of alkenes	15-11	ALKENE-AMINES	
hydrogenation of alkynes	15-11	rearrangement of alkene-ammonium salts	18-35
hydrogenation of aromatic compounds	15-13		
inorganic esters + RM	10-61	ALKENE-CARBOXYLIC ACIDS	
insertion by carbenes	12-21	Claisen rearrangement	18-33
pyrolysis of peroxides	17-37	rearrangement of alkene-esters	18-33
radical addition to alkenes	15-29		
radical coupling of alkanes	14-14	ALKENE-KETONES	
radical cyclization of alkenes	15-30	Claisen rearrangement	18-33
reduction dithioketals	10-71	rearrangement of allyl vinyl ethers	18-33
reduction of acyl halides	19-59		
reduction of alkyl halides	19-53	ALKENE-THIOETHERS	
reduction of carbonyls to methylene	19-61	rearrangement of alkene sulfonium salts	18-35
reduction of nitro compounds	19-67		
reduction of silanes	19-52	ALKENES	
reduction of sulfonate esters	19-57	1,3-elimination of diols	17-25
reduction of sulfur compounds	19-70	1,3-elimination of halo-amines	17-25
reduction of thioethers	14-27	1,3-elimination of halohydrins	17-25
reduction of thiols	14-27	addition of alkanes to alkynes	15-18
reduction of thiols	19-70	addition of alkenes to alkenes	15-20
reduction of xanthate esters	19-58		
reductive cleavage	15-15		
of cyclopropanes			
reductive cleavage of ethers	19-56		

aldehydes or ketones + active H compounds	16-38	cleavage of ethers	17-02
alkene metathesis	18-37	cleavage of vinyl ethers	17-02
alkenes + arylboronic acids	13-10	conjugated addition of allylsilanes	15-26
alkenes + aryldiazonium compounds	13-10	deacyloxylation	19-59
alkenes + carbenes	15-64	decarbonylation of acyl halides	17-17
alkenes + carbocations	12-20	decarboxylation of hydroxy-carboxylic acids	17-26
alkynes + aryl halides + RM (M = metal)	15-22	dehydration of alcohols	17-01
alkynes + metals or metal hydrides	15-12	dehydrogenation	19-02
allylic halides + metals	10-56	deoxygenation of 1,2-diols	17-18
allylic silanes + esters	10-60	dialkoalkanes + aldehydes	15-64
base induced elimination of halo-sulfones	17-20	dimerization of alkyl halides	19-32
base induced elimination of sulfonyl hydrazones	17-11	elimination of 1,2-dihalides	17-22
base-induced elimination of ammonium salts	17-08	elimination of boranes	17-15
base-induced elimination of halides	17-13	elimination of halo-ethers	17-24
base-induced elimination of sulfonate esters	17-06	enamines + boranes	15-16
base-induced elimination of sulfonyl halides	17-14	esters + organometallics	10-60
bis-decarboxylation of dicarboxylic acids	19-13	extrusion from oxathiolanes	17-38
by decarboxylation	12-40	extrusion of CO from cyclic ketones	17-35
by McMurry coupling	19-77	from episulfones	16-48
by Peterson alkenylation	16-41	from bis(xanthates)	17-18
by the Diels–Alder reaction	15-60	from boranes	10-59
by the ene reaction	15-23	from carbenes	12-21
by the Heck reaction	13-10	from dienes	18-37
by the heteroatom Diels–Alder reaction	15-61	from epoxides or thiiranes	17-03
by the Horner–Wadsworth–Emmons reaction	16-44	from imines	16-44
by the Knoevenagel reaction	16-38	hydroboration of alkynes	18-25
by the Ramberg–Bäcklund reaction	17-20	hydrogenation of alkynes	15-11
by the Sakurai reaction	15-26	hydrogenation of aromatic compounds	15-13
by the Wittig reaction	16-44	isomerization of double bonds	15-01
by [2+2]-cycloaddition	15-63	ketones or aldehydes + bis-Grignards	16-24
by [3+2]-cycloaddition	15-59	migration of boranes	12-02
		migration of double bonds	12-02
		nitrosation of aziridines	17-21
		organometallics + ketones	16-25
		organometallics + tosylhydrazones	16-38
		other cycloaddition reactions	15-66
		oxidative decarboxylation of carboxylic acids	19-12

Petasis alkenylation	16-45	ALKYNES	
protonolysis of vinyl boranes	18-25	alkyl halides + alkyne anions	10-74
protonolysis of vinyl boranes	18-26	alkyl halides + propargylic RM	10-57
pyrolysis of amine oxides (Cope)	17-09	alkynes + arylodonium salts	13-13
pyrolysis of ammonium salts (Hofmann)	17-07	alkynes + boranes	18-26
pyrolysis of β -lactones	17-26	aryl halides + alkyne-M (M = a metal)	13-13
pyrolysis of esters	17-04	aryl halides + alkynes	10-74
pyrolysis of hydroxy-alkenes	17-32	base-induced elimination	17-16
pyrolysis of sulfones	17-12	of dihalo compounds	
pyrolysis of sulfoxides	17-12	base-induced elimination	17-13
pyrolysis of thionocarbonates	17-19	of halides	
pyrolysis of xanthates (Chugaev)	17-05	by Sonogashira coupling	13-13
reduction of alcohols	19-54	dimerization of dihalides	19-32
reduction of amines	19-67	elimination of alkenes	17-16
reduction of carboxylic esters	19-65	hypervalent iodine + alkyne-M (M = a metal)	12-26
reduction of enamines	19-67	metathesis of	18-37
reduction of nitriles	19-66	pyrolysis of	17-07
reduction of thiiranes	19-35	bis(ammonium salts)	
reduction of thiophene derivatives	19-70	pyrolysis of thiirene dioxides	17-20
reduction of vinyl halides	19-53	pyrolysis of ylids	17-10
reduction of vinyl imines	19-61	ALLENES	
reductive coupling	19-77	base-induced rearrangement	18-03
of aldehydes or ketones		of halocyclopropanes	
reductive coupling of epoxides	19-35	by Claisen rearrangement	18-33
sigmatropic carbon migration	18-30	by the Wittig reaction	16-44
sigmatropic H migration	18-29	Cope rearrangement of di-yens	18-32
silyl-organometallics + aldehydes or ketones	16-41	elimination of dihalides	17-22
Tebbe alkenylation	16-45	propargylic esters + organocuprates	10-60
vinyl boranes + halogen/base	18-25	reduction of alkynes	19-53
vinyl halides + arylboronic acids	13-10	ALLOPHANATES	
vinyl-cyclopropane rearrangement	18-31	carbamates + isocyanates	16-08
vinyl-X + alkyl(aryl)boronic acids	12-15	AMIDE-ESTERS	
Wagner–Meerwein rearrangement of alcohols	18-01	aziridines + amides	10-14
Wagner–Meerwein rearrangement of halides	18-01	AMIDES	
ALKYNE-ALCOHOLS		acyl halides + ammonia or amines	16-72
addition of alkynes to carbonyls	16-25	addition of organometallics to isocyanates	16-33

alcohols + cyanogen halides	16-09	<i>N</i> -arylation	10-41
aldehydes + ammonia + oxidant	14-11	nitriles + alcohols	16-91
alkanes + nitriles	14-12	nitriles + amines	16-21
alkenes + amides	15-09	oxidation of methylene	19-17
alkenes + nitriles	16-91	in amines	
alkyl halides + amides	10-41	oxidation of methylene	19-17
alkylation of amides	19-73	in lactams	
amides + aldehydes	10-41	oximes + halogenating	18-17
amides + amines	16-76	or oxidizing agents	
amines + CO + alkenes	15-36	pyrolysis of imino esters	18-42
amines + CO	12-53	rearrangement of oximes	18-17
amines + haloformates	10-53	reduction of imides	19-64
amines + organoiron	10-77	transamidation	16-70
compounds			
amines + vinyl esters	16-75	AMIDINES	
anhydrides + ammonia	16-73	ketenimines + amines	15-08
or amines		nitriles + ammonia or amines	16-21
aromatic compounds + amides	11-22		
aromatic compounds +	11-06	AMINE OXIDES	
hydroxamic acids		oxidation of amines	19-29
aromatic compounds +	11-21		
isocyanates		AMINES	
aryl halides + amides	10-41	addition of organometallics	16-31
aryl halides + amides	13-05	to C=N compounds	
aryl halides, DMF and POCl ₃	11-21	addition of silanes to C=N	16-31
by Beckmann rearrangement	18-17	alkenes + amines or ammonia	15-08
by Michael addition	15-24	alkyl halides + amines	10-31
by the Willgerodt reaction	19-84	alkylation of amines	10-31
carboxylic acids +	16-74	alkylation of formamidines	10-71
amino-boranes		alkylation of nitroso amines	10-71
carboxylic acids and ammonia	16-74	amides + organometallic	16-82
or amines		compounds	
carboxylic esters + ammonia	16-75	amination of active methylene	12-12
or amines		compounds	
cleavage of ketones	12-46	amination of alkanes	10-39
condensation of methyl ketones	19-84	amination of alkanes	12-12
from alcohols	10-41	amination of methylene	19-16
hydrolysis of isonitriles	16-97	amines + aryl halides	13-05
hydrolysis of nitriles	16-04	amines + diaryliodonium	11-06
imines + borane + CO	12-33	compounds	
insertion of acyl nitrenes	12-13	amines + diazo compounds	10-34
insertion of diazo amides	12-21	aminomethylation of aromatic	11-22
ketenes + amines	15-08	compound	
ketones + HN ₃	18-16	aromatic compounds +	13-18
<i>N</i> -alkylation	10-41	amide bases	

aromatic compounds + aryl azides	11-06	rearrangement of ammonium salts	13-31
aromatic compounds + halo-amines	11-06	rearrangement of ammonium salts	18-21
aromatic compounds + hydrazoic acid	11-06	rearrangement of aryl hydroxylamines	13-32
aryl halides + alkyl organometallics	13-05	reduction nitroso compounds	19-47
aryl halides + hydroxylamine- <i>O</i> -sulfonic acid	18-15	reduction of amine oxides	19-68
azides + haloboranes	12-32	reduction of amines	19-64
aziridines + RM	10-66	reduction of azides	19-50
boranes + ammonia + NaOCl	12-32	reduction of azo compounds	19-74
boranes + chloramine	12-32	reduction of azoxy compounds	19-74
by the Stevens rearrangement	18-21	reduction of C=N compounds	19-42
by transamination	10-33	reduction of hydrazines	19-74
Curtius rearrangement	18-14	reduction of hydroxylamines	19-47
cyclization of halo-amines	18-40	reduction of isocyanates	19-51
dealkylation of amines	19-73	reduction of isothiocyanates	19-51
displacement of cyano	10-62	reduction of lactams	19-64
diynes + amines	15-08	reduction of nitriles	19-43
enamines + boranes	15-16	reduction of nitriles	19-45
from alcohols	10-31	reduction of nitro compounds	19-45
from alcohols	10-32	reduction of nitroso-amines	19-51
from amides	18-13	reduction oximes	19-48
from amines	10-33	reductive alkylation of aldehydes or ketones	16-17
from amino-nitriles	10-62	Schmidt reaction	18-16
from boranes	10-31		
from cyanohydrins	10-32	AMINO-ACIDS	
from ethers	10-32	lactones + ammonia or amines	16-75
from halo-amines	10-31	AMINO-ALCOHOLS :	
Hofmann rearrangement	18-13	see hydroxy-amines	
hydrolysis of isocyanates	18-13	AMINO-ALDEHYDES	
hydrolysis of isocyanates	18-15	aldehydes + C=N compounds	16-31
hydrolysis of isocyanates	18-16	AMINO-ESTERS	
hydroxylamines + alkyl organometallics	12-32	diazoesters + amines	15-64
insertion of nitrenes	12-13	AMINO-ETHERS	
Lossen rearrangement	18-15	aziridines + alcohols	10-14
Michael addition	15-31	AMINO-KETONES	
with <i>N</i> nucleophiles		base-induced rearrangement of sulfonyl oximes	18-12
phenols + amines	13-06	ketones + HCHO + amines	16-19
or ammonia		Mannich reaction	16-19
radical addition to C=N compounds	16-56		

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