Appendix A
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," etc., 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 shall examine the literature of organic chemistry, confining our attention chiefly to the results of laboratory work, rather than those of industrial organic chemistry.[1] 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* 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.

PRIMARY SOURCES

Journals

For well over a hundred 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. Of course, this is still a large number, especially since some are published weekly and some semimonthly, but it is considerably smaller than the total number of journals (perhaps as high as 10,000) that publish chemical articles.

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

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 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.

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.

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, and even such traditionally German or French journals as *Chemische Berichte, Liebigs Annalen der Chemie*, and *Bulletin de la Société Chimique de France* now publish some papers in English. Most of the articles published in other languages have summaries printed in English also. Furthermore, the second most important language (in terms of the number of organic chemical papers published) is Russian, and most of these papers are available in English translation, though in most cases, six months to a year later. A considerable number of important papers are published in German and French; these are generally not available in translation, so that the organic chemist should have at least a reading knowledge of these languages. An exception is 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 even more important for the older literature. Before about 1920, more than half of the important chemical papers were in these languages. It must be realized that the original literature is never obsolete. 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 papers[3] 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.

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 "Synopses," 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. For some years, the American Chemical

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

[3]In Table A.1 notes are counted as papers.

TABLE A.1 A list of the more important current journals that publish original papers in organic chemistry, listed in alphabetical order of *Chemical Abstracts* abbreviations, which are indicated in boldface. Also given are the year of founding, number of issues per year as of 1991, and whether the journal primarily publishes papers (P), communications (C), or both

No.	Name	Papers or communications	Issues per year
1	**Acta Chem**ica **Scand**inavica (1947)	P	10
2	**Angew**andte **Chem**ie (1888)[4]	C[5]	12
3	**Aust**ralian **J**ournal of **Chem**istry (1948)	P	12
4	**Bioorg**anic **Chem**istry (1971)	P[5]	4
5	**Bioorg**anic & **Med**icinal **Chem**istry **Lett**ers (1991)	C	12
6	**Bull**etin of the **Chem**ical **Soc**iety of **Jap**an (1926)	P	12
7	**Bull**etin des **Soc**iétés **Chim**ique **Belg**es (1887)	P	12
8	**Bull**etin de la **Soc**iété **Chim**ique de **Fr**ance (1858)	P[5]	6
9	**Can**adian **J**ournal of **Chem**istry (1929)	PC	12
10	**Carbohydr**ate **Res**earch (1965)	PC	22
11	**Chem**ische **Ber**ichte (1868)[6]	P	12
12	**Chem**istry and **Ind**ustry **(London)** (1923)	C	24
13	**Chem**istry **Lett**ers (1972)	C	12
14	**Chimia** (1947)	C[5]	12
15	**Collect**ion of **Czech**oslovak **Chem**ical **Commun**ications (1929)	P	12
16	**Dokl**ady **Akad**emii **Nauk SSSR** (1922)[4]	C	36
17	**Gazz**etta **Chim**ica **Ital**iana (1871)	P	12
18	**Helv**etica **Chim**ica **Acta** (1918)	P	8
19	**Heteroat**om **Chem**istry (1990)	P	6
20	**Heterocycles** (1973)	C[5]	12
21	**Int**ernational **J**ournal of **Chem**ical **Kinet**ics (1969)	P	12
22	**Isr**ael **J**ournal of **Chem**istry (1963)	P[7]	4
23	**Izv**estiya **Akad**emii **Nauk SSSR, Ser**iya **Khim**icheskaya (1936)[4]	PC	12
24	**J**ournal of the **Am**erican **Chem**ical **Soc**iety (1879)	PC	26
25	**J**ournal of **Chem**ical **Res**earch, **Synop**ses (1977)	P	12
26	**J**ournal of the **Chem**ical **Soc**iety, **Chem**ical **Commun**ications (1965)	C	24
27	**J**ournal of the **Chem**ical **Soc**iety, **Perkin Trans**actions **1**: Organic and Bio-Organic Chemistry (1841)[8]	PC	12
28	**J**ournal of the **Chem**ical **Soc**iety, **Perkin Trans**actions 2: Physical Organic Chemistry (1841)[8]	P	12

[4]These journals are available in English translation; see Table A.2.
[5]These journals also publish review articles regularly.
[6]Former title: **Ber**ichte der deutschen chemischen Gesellschaft.
[7]Each issue of this journal is devoted to a specific topic.
[8]Beginning with 1966 and until 1971, *J. Chem. Soc.* was divided into three sections: *A*, *B*, and *C*. Starting with 1972, Section *B* became *Perkin Trans. 2* and Section *C* became *Perkin Trans. 1*. Section *A* (Physical and Inorganic Chemistry) was further divided into *Faraday* and *Dalton Transactions*.

TABLE A.1 *(Continued)*

No.	Name	Papers or communications	Issues per year
29	Journal of **Fluorine Chem**istry (1971)	PC	12
30	Journal of **Heterocyclic Chem**istry (1964)	PC	12
31	Journal of the **Indian Chem**ical **Soc**iety (1924)	P	12
32	Journal of **Med**icinal **Chem**istry (1958)	PC	12
33	Journal of **Mol**ecular **Struc**ture (1967)	PC	16
34	Journal of **Organomet**allic **Chem**istry (1963)	PC	48
35	Journal of **Org**anic **Chem**istry (1936)	PC	26
36	Journal of **Photochem**istry and **Photobiol**ogy, **A**: Chemistry (1972)	P	12
37	Journal of **Phys**ical **Org**anic **Chem**istry (1988)	P	12
38	Journal für **Prak**tische **Chem**ie (1834)	P	6
39	**Khim**iya **Geterotsikl**icheskikh **Soedin**enii (1965)[4]	P	12
40	**Liebigs Ann**alen der **Chem**ie (1832)	P	12
41	**Mendeleev Commun**ications (1991)	C	8
42	**Metalloorg**anicheskaya **Khim**iya (1988)[4]	PC	6
43	**Monatsh**efte für **Chem**ie (1870)	P	12
44	**New** Journal of **Chem**istry (1977)[9]	P	11
45	**Organometallics** (1982)	PC	12
46	**Org**anic **Mass Spectrom**etry (1968)	PC	12
47	**Org**anic **Prep**arations and **Proced**ures **Int**ernational (1969)	P[5]	6
48	**Photochem**istry and **Photobiol**ogy (1962)	P[5]	12
49	**Polish** Journal of **Chem**istry (1921)[10]	PC	12
50	**Pure** and **Appl**ied **Chem**istry (1960)	[11]	12
51	**Rec**ueil des **Trav**aux **Chim**iques des **Pays-Bas** (1882)	PC	12
52	**Res**earch on **Chem**ical **Intermed**iates (1973)[12]	P[5]	6
53	**Sulf**ur **Lett**ers (1982)	C	6
54	**Synlett** (1989)	C[5]	12
55	**Synth**etic **Commun**ications (1971)	C	22
56	**Synthesis** (1969)	P[5]	12
57	**Tetrahedron** (1958)	P[5]	48
58	**Tetrahedron: Asymmetry** (1990)	PC	12
59	**Tetrahedron Lett**ers (1959)	C	52
60	**Zh**urnal **Obshch**ei **Khim**ii (1869)[4]	PC	12
61	**Zh**urnal **Org**anicheskoi **Khim**ii (1965)[4]	PC	12

Society journals, including *J. Am. Chem. Soc.* and *J. Org. Chem.*, have provided supplementary material for some of their papers. This material is available from the Microforms and Back Issues Office at the ACS Washington office, either on microfiche or as a photocopy. These practices have not yet succeeded in substantially reducing the total volume of the world's primary chemical literature.

[9]Before 1987 this journal was called **Nouveau** Journal de **Chim**ie.
[10]Before 1978 this journal was called **Rocz**niki **Chem**ii.
[11]*Pure Appl. Chem.* publishes IUPAC reports and lectures given at IUPAC meetings.
[12]Before 1989 this journal was called **Rev**iews of **Chem**ical **Intermed**iates.

TABLE A.2 Journals from Table A.1 available in English translation. The numbers are keyed to those of Table A.1. The year of first translation is given

2	**Angew**andte **Chem**ie, **Int**ernational **Ed**ition in **Engl**ish (1962)
16	**Dokl**ady **Chem**istry (**Engl**ish **Transl**ation) (1956)
23	**Bull**etin of the **Acad**emy of **Sci**ences of the **USSR, Div**ision of **Chem**ical **Sci**ence (1952)
39	**Chem**istry of **Heterocyclic Comp**ounds (**Engl**ish **Transl**ation) (1965)
42	**Organomet**allic **Chem**istry in the **USSR** (1988)
60	Journal of **Gen**eral **Chem**istry of the **USSR** (1949)
61	Journal of **Org**anic **Chem**istry of the **USSR** (1949)

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 to 30%) are chemical patents. Chemical patents are part of the chemical literature, and both U.S. and foreign patents are regularly abstracted by *Chemical Abstracts*. 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, D.C., 20231. In addition, *Chemical Abstracts* lists, in the introduction to the first issue of each volume, instructions for obtaining patents from 26 countries.

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 he or she 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. In general, however, the laboratory chemist must be more wary of patents than of papers.

SECONDARY SOURCES

Journal articles and patents contain virtually all of the original work in organic chemistry. However, if this were all—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 he or she does not normally read. There are two "title" publications covering the whole of chemistry. One of these, *Current Contents Physical, Chemical & Earth Sciences*,[13] which began in 1967 and appears weekly, contains the contents pages of all issues of about 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. *Current Contents* is also available on computer discs, with "keywords"—words taken from the title and the interior of the paper. The discs can be searched for the keywords, allowing the user to find papers containing specific topics of interest.

The other "title" publication is *Chemical Titles*, published by Chemical Abstracts Service. This biweekly publication, begun in 1961, lists, in English, all titles from more than 700 journals, all in the field of chemistry. The most useful aspect of this publication is the way the titles are given. They are listed in alphabetical order of *every word in the title*, except for such words as "the," "of," "investigation," "synthesis," etc. (each issue contains a list of words prevented from indexing). This means that a title containing seven significant words is listed seven times. These words are also called "keywords". Furthermore, at each listing are given the words that immediately precede and follow the keyword. In the second section of each issue (called the Bibliography) the complete titles and the authors are given. Incidentally, this Bibliography duplicates, for the journals they both cover, the listings in *Current Contents Physical, Chemical, & Earth Sciences*, since the complete contents of journals are given in order of page number. Each issue of *Chemical Titles* has an author index, covering all authors, not just the first author. Addresses are not given.

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. From the earliest days of organic chemistry, abstracts of papers have been widely available, often as sections of journals whose principal interests lay elsewhere.[14] 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-

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

[14]For 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 *Ber.* also did so.

speaking chemists. The other is *Chemical Abstracts*. 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.[15] Approximately 18,000 journals are covered, in many languages. In addition, *CA* publishes abstracts of every patent of chemical interest from 18 countries, including the United States, United Kingdom, Germany, and Japan, as well as many patents from eight additional countries. *CA* lists and indexes but does not abstract review articles and books. The abstracts currently appear in 80 sections, of which sections 21 to 34 are devoted to organic chemistry, under such headings as Alicyclic Compounds, Alkaloids, Physical Organic Chemistry, Heterocyclic Compounds (One Hetero Atom), etc. Each abstract of a paper begins with a heading that gives (1) the abstract number;[16] (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);[17] (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. *CA* abstracts only the first patent, but 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 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.[18] *CA* 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 ten-year (decennial) indexes, but the volume of information has made five-year indexes necessary since 1956. Collective indexes so far published are shown in Table A.3. Thus a user of the indexes at the time of this writing would consult the collective indexes through 1986 and the semiannual indexes thereafter. The 12th collective index (covering 1987 through 1991) is scheduled to appear in 1992.

[15]For a guide to the use of *CA*, see Schulz *From CA to CAS ONLINE*; VCH: New York, 1988.

[16]Beginning in 1967. See p. 1247.

[17]These abbreviations are changed from time to time. Therefore the reader may notice inconsistencies.

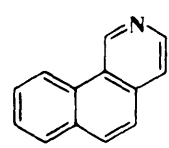
[18]It is possible to subscribe to *CA Selects*, which provides copies of all abstracts within various narrow fields, such as organofluorine chemistry, organic reaction mechanisms, organic stereochemistry, etc.

TABLE A.3 *CA* collective indexes so far published

Coll. index	Subject General subject	Chemical substance	Author	Formula	Patents
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

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 he or she 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 he or she would find the sublisting $C_5N—C_6—C_6$ (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 $C_5N—C_6—C_6$. A search of the chemical substance index under these names will give all references to these ring systems that have 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., 4327^5, 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 C_3 compounds are listed before any C_4 compound; all C_5H_7 compounds before any C_5H_8 compound; $C_7H_{11}Br$ before $C_7H_{11}N$; $C_9H_6N_4S$ before C_9H_6O, etc. Deuterium and tritium are represented by D and T and treated alphabetically, e.g., C_2H_5DO after C_2H_5Cl and before C_2H_5F or C_2H_6.

Since 1965, *CA* has assigned a Registry Number to each unique chemical substance. 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. Registry Numbers are primarily for computer use. All numbers so far have been published with the *CA* preferred names in a multivolume "Registry Handbook."

For abstracts printed since 1967 (the eighth collective period and later) *CA* can be searched by computer online. For a discussion of online searching see pp. 1260-1266.

Although *CA* and *Referativnyi Zhurnal, Khimya* are currently the only chemical abstracting publications that cover the entire field of chemistry, 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.[19] *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. For

[19]An "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).

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, refractive index, etc.; 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.[20] 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 system too elaborate to discuss fully here.[21] The compounds are divided into three divisions which are further subdivided into "systems":

	Division	Volumes	System numbers
I.	Acyclic compounds	1–4	1–449
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 Ergänzungwerk*) 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,[22] except that supplements 3 and 4 are combined for vols. 17 to 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

[20]For a discussion of how data are processed for inclusion in Beilstein, see Luckenbach; Ecker; Sunkel *Angew. Chem. Int. Ed. Engl.* **1981**, *20*, 841-849 [*Angew. Chem. 93*, 876-885].

[21]For descriptions of the Beilstein system and directions for using it, see Sunkel; Hoffmann; Luckenbach *J. Chem. Educ.* **1981**, *58*, 982; Luckenbach *CHEMTECH* **1979**, 612-621. 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 *A Manual for the Use of Beilstein's Handbuch der Organischen Chemie*; Springer: New York, 1976. An older work, which many students will find easier to follow, is by Huntress *A Brief Introduction to the Use of Beilstein's Handbuch der Organischen Chemie*, 2nd ed.; Wiley: New York, 1938.

[22]In 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.

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 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 to 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.[23] Similar index volumes, covering all four supplements, have been issued for the other volumes, 2 to 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. 1247).

There is also a fourth division of Beilstein (systems 4721 to 4877) that covers natural products of uncertain structure: rubbers, sugars, etc. 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 online.

Compendia and 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 fifth edition of "Heilbron's Dictionary of Organic Compounds," J. Buckingham, Ed., 7 vols., Chapman and Hall, London, 1982, contains brief listings of more than 150,000

[23]Most page number entries in the combined indexes contain a letter, e.g., $CHBr_2Cl$ 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, etc. No letters are given for the fourth supplement.

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, hetero atoms, and *CA* Registry Numbers. Annual supplements, with cumulative indexes, have appeared since 1983. A similar work, devoted to organometallic compounds, is "Dictionary of Organometallic Compounds," 3 vols. with supplements, published by Chapman and Hall beginning in 1984. Another, "Dictionary of Steroids," 2 vols., 1991, is also published by Chapman and Hall.

2. A multivolume compendium of physical data is Landolt-Börnsteins'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 (71st ed., 1990-91), is a valuable repository of data quickly found. For organic chemists the most important table is "Physical Constants of Organic Compounds," 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," 13th ed., McGraw-Hill, New York, 1985. Another such handbook, but restricted to data of interest to organic chemists, is Dean, "Handbook of Organic Chemistry," McGraw-Hill, New York, 1987. 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, 1955-1961 lists many physical properties of more than 1000 organic compounds.

6. Physical properties of thousands of organometallic compounds, with references, are collected in four 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.

7. The "Merck Index," 11th ed., Merck and Company, Rahway, NJ, 1989, 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, but the 11th edition omits this list.

8. There are two publications that list properties of azeotropic mixtures. Timmermans, "The Physico-Chemical 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 no. 6 and no. 35, American Chemical Society, Washington, 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, Rahara 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. 1246). 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 more than 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 to 9 contain indexes of spectral peaks for ir, uv, 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 volume 10).

14. The "Aldrich Library of Infrared Spectra," 3rd ed., Aldrich Chemical Company, Milwaukee, WI, 1981, by Pouchert contains more than 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 about 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; e.g., the titles of some recent reviews are "Preparation, Properties, and Reactions of Carbonyl Oxides,"[24] "Enantioselective Addition of Organometallic Reagents to Carbonyl Compounds: Chirality Transfer, Multiplication, and Amplification,"[25] 1,3-Dipolar Cycloadditions of Diazoalkanes to some Nitrogen Containing Heteroaromatic Systems,"[26] and "Alkyl and Aryl-Substituted Main-Group Metal Amides."[27] 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.4. Some of the journals listed in Table A.1, for example, the *Bull Soc. Chim. Fr.* 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 hard-bound. 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.5 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 all review articles in the field of organic chemistry that have appeared in the preceding three 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.

TABLE A.4 Review journals, with year of founding and issues per year as of 1991

Accounts of **Chem**ical **Res**earch (1968)	12
Aldrichimica Acta (1968)	4
Angewandte **Chem**ie (1888)	12
and its English Translation:	
Angewandte **Chem**ie, **I**nternational **Ed**ition in **Engl**ish (1962)	12
Chemical **Rev**iews (1924)	8
Chemical **Soc**iety **Rev**iews (1947)[28]	4
Heterocycles (1973)	12
Natural **Prod**uct **Rep**orts (1984)	6
Soviet Scientific Reviews, Section B, Chemistry Reviews (1979)	Irreg.
Sulfur Reports (1980)	6
Synthesis (1969)	12
Tetrahedron (1958)	48
Topics in **Curr**ent **Chem**istry (1949)[29]	Irreg.
Uspekhi **Khim**ii (1932)	12
and its English translation: **Russ**ian **Chem**ical **Rev**iews (1960)	12

[24]Bunnelle *Chem. Rev.* **1991,** *91*, 335-362.
[25]Noyori; Kitamura *Angew. Chem. Int. Ed. Engl.* **1991,** *30*, 49-69 [*Angew. Chem. 103* 34-55].
[26]Stanovnik *Tetrahedron* **1991,** *47*, 2925-2945.
[27]Veith *Adv. Organomet. Chem.* **1990,** *31*, 269-300.
[28]Successor to *Quarterly Reviews* (abbreviated as *Q. Rev., Chem. Soc.*).
[29]Formerly called **Fortschritte** der **Chem**ischen **Forsch**ung.

TABLE A.5 Irregularly Published Serial Publications

Advances in **Carbocation Chem**istry	**Fortshr**itte der **Chemie Org**anischer **Naturst**offe
Advances in **Carbohydr**ate **Chem**istry and **Biochem**istry	**Isot**opes in **Org**anic **Chem**istry
Advances in **Catal**ysis	**Mol**ecular **Struct**ure and **Energ**etics
Advances in **Cycloadd**ition	**Org**anic **Photochem**istry
Advances in **Free Radical Chem**istry	**Organomet**allic **React**ions
Advances in **Heterocyclic Chem**istry	**Org**anic **React**ions
Advances in **Metal-Org**anic **Chem**istry	**Org**anic **Synth**esis: **Theory** and **Appl**ications
Advances in **Mol**ecular **Model**ing	**Prog**ress in **Heterocyclic Chem**istry
Advances in **Organomet**allic **Chem**istry	**Prog**ress in **Macrocyclic Chem**istry
Advances in **Oxygenated Processes**	**Prog**ress in **Phys**ical **Org**anic **Chem**istry
Advances in **Photochem**istry	**React**ive **Int**ermediates (Plenum)
Advances in **Phys**ical **Org**anic **Chem**istry	**React**ive **Int**ermediates (Wiley)
Advances in **Protein Chem**istry	**Surv**ey of **Prog**ress in **Chem**istry
Advances in **Theor**etically **Interesting Mol**ecules	**Top**ics in **Phys**ical **Organomet**allic **Chem**istry
Fluorine Chemistry **Rev**iews	**Top**ics in **Stereochem**istry

Another publication is the "Index of Reviews in Organic Chemistry," complied by Lewis, Chemical Society, London, a classified listing of review articles. The first volume, published in 1971, lists reviews from about 1960 (in some cases much earlier) to about 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 Walton[30] and by Bruce.[31] A similar list for heterocyclic chemistry is found in articles by Katritzky and others.[32] See also the discussion of the *Index of Scientific Reviews*, p. 1267.

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).

[30]Smith; Walton *Adv. Organomet. Chem.* **1975,** *13*, 453-558.
[31]Bruce *Adv. Organomet. Chem.* **1972,** *10*, 273-346, **1973,** *11*, 447-471, **1974,** *12*, 380-407.
[32]Belen'kii *Adv. Heterocycl. Chem.* **1988,** *44*, 269-396; Katritzky; Jones *Adv. Heterocycl. Chem.* **1979,** *25*, 303-391; Katritzky; Weeds *Adv. Heterocycl. Chem.* **1966,** *7*, 225-299.

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, 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 closings and bond breakings. 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. Each issue deals with about 20 papers, and also includes a review article.

2. The Institute for Scientific Information (ISI), besides publishing *Current Contents* (p. 1244) and the *Science Citation Index* (p. 1266), 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 more than 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 unisolated intermediates. 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, 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, e.g., hydrocarbons, oxygen compounds, nitrogen compounds, etc. 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, 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.

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 more than 20 functional groups have appeared so far, including books on alkenes, cyano compounds, amines, carboxylic acids and esters, quinones, etc.

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 but valuable reference books for graduate students and practicing chemists.

Baker and Engel, "Organic Chemistry," West Publishing Co., St. Paul, MN, 1992.

Carey, "Organic Chemistry," 2nd ed., McGraw-Hill, New York, 1992.

Carey and Sundberg, "Advanced Organic Chemistry," 2 vols., Plenum, New York, 3rd. ed., 1990.

Carruthers, "Some Modern Methods of Organic Synthesis," 3rd ed., Cambridge University Press, Cambridge, 1986.

Ege, "Organic Chemistry," 2nd ed., D.C. Heath, New York, 1989.

Fessenden and Fessenden, "Organic Chemistry," 4th ed., Brooks/Cole, Monterey, CA, 1990.

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, New York, 1987.

Jones, "Physical and Mechanistic Organic Chemistry," 2nd ed., Cambridge University Press, Cambridge, 1984.

Loudon, "Organic Chemistry," 2nd ed., Benjamin/Cummings, Menlo Park, CA, 1988.

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

McMurry, "Organic Chemistry," 2nd ed., Brooks/Cole, Monterey, CA, 1988.

Maskill, "The Physical Basis of Organic Chemistry," Oxford University Press, Oxford, 1985.

Morrison and Boyd, "Organic Chemistry," 6th ed., Prentice-Hall, Englewood Cliffs, NJ, 1992.

Pine, "Organic Chemistry," 5th ed., McGraw-Hill, New York, 1987.

Ritchie, "Physical Organic Chemistry," 2nd ed., Marcel Dekker, New York, 1989.

Solomons, "Organic Chemistry," 5th ed., Wiley, New York, 1992.

Streitwieser, Heathcock, and Kosower,"Introduction to Organic Chemistry," 4th ed., Macmillan, New York, 1992.

Sykes, "A Guidebook to Mechanism in Organic Chemistry," 6th ed., Longmans Scientific and Technical, Essex, 1986.

Vollhardt, "Organic Chemistry," W.H. Freeman, San Francisco, 1987.
Wade, "Organic Chemistry," 2nd ed., Prentice-Hall, Englewood Cliffs, NJ, 1991.

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**

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 to VII and annual vols. 65 to 68) into eleven 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 which 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. Fourteen 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 to 12, by Smith and Fieser, was published in 1990.

3. "Comprehensive Organic Transformations," by Larock, VCH, New York, 1989, 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.

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, etc. 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. Seven volumes have been published so far (1971 and 1974, edited by Harrison and Harrison; 1977, edited by Hegedus and Wade; 1980 and 1984, edited by Wade; 1988 and 1992, edited by Smith).

7. "The Vocabulary of Organic Chemistry," by Orchin, Kaplan, Macomber, Wilson, and Zimmer, Wiley, New York, 1980, presents definitions of more than 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 online searching.[32a]

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

[32a]For a monograph that covers both online searching and searches using printed materials, see Wiggins *Chemical Information Sources*; McGraw-Hill: New York, 1991.

spectrum, or some other property. Someone who wants all the information that has ever been published on any compound begins by consulting the formula indexes in Beilstein (p. 1249). At this time there are two ways to do this. (1) The formula index to the second supplement (Vol. 29, see p. 1249) 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. 1249 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.[33] 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.[34] 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:* 1957-1961; 1962-1966; 1967-1971; 1972-1976; 1977-1981; 1982-1986; 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 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 a 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, etc., 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 eluent in a common procedure.

[33]Compounds 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. 21), but they may also be found by consulting *CA* indexes beginning with the sixth collective index, or by using Beilstein online.

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

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 (p. 1261). However, if one lacks access to these, one may consult *Chemical Titles* and the keyword index (p. 1244) 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* (p. 1254); one consults the formula indexes. However, these methods are far from complete. *Index Chemicus* lists primarily new compounds, those which would not have been found in the earlier search. As for *Chemical Titles*, the compound can be found only if it is mentioned in the title. 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 *CA* online.

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. 1250), in the "Dictionary of Organic Compounds" (p. 1249), or in one of the other compendia listed in this chapter, most of which give references to the original literature.

Other Searches[35]

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 —C(NH_2)=N— absorbs in the ir, is dependent on his or her 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 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," etc., 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 about 1920), recourse may be made to *Chemisches Zentralblatt* (p. 1247) and the abstracts in the *Journal of the Chemical Society* (p. 1247).

Literature Searching Online[32a]

Online searching means using a computer terminal to search a *database*. Although databases in chemistry are available from several organizations, by far the most important such or-

[35]This discussion is necessarily short. For much more extensive discussions, consult the books in Refs. 1 and 15.

ganization is STN International (The Scientific & Technical Information Network), which is 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 *CA* online, which is one of the databases available from STN. One thing that must be remembered is that *CA* online is complete only from 1967 to the present,[36] 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 shall see, one can do kinds of searches online that are simply not possible using only the printed volumes. Furthermore, the online files are updated every two weeks, so that one will find all the abstracts online well past the appearance of the latest semiannual indexes, often even before the library has received the latest weekly printed issue of *CA*. *CA* 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[37] (*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. *CA* online has two major files, *the CA File* and *the Registry File*.[38] These are so different that we discuss them separately.

The CA File

This file is accessed with the command FILE CA. Once in the file, the user uses the command SEARCH (or SEA or S)[39] to look for references to specific terms. For example, one may type SEA SEMIPINACOL. On the screen will appear something like

L1 4 SEMIPINACOL

The L1 means that this is line one. Future answers from the system will number the lines in consecutive order. The 4 means that the system has four abstracts that contain the word semipinacol. The word may be in the title, an index entry, or a keyword. The search term may be the name of a compound, which means that individual compounds can be searched for in this way. If the name used is the *CA* indexing name, all the abstracts mentioning that compound will be retrieved. However, common names or other names can also be searched (e.g., catechol), and if they are mentioned in the title of the paper, or, for example as a keyword, those abstracts will be retrieved.

Compounds can also be searched for by using the Registry Number, e.g.,

SEARCH 126786-44-3

Let us return to the example of semipinacol. The system told us there were four abstracts for this term. We may now see these abstracts by using the display command (DISPLAY or DIS or D), e.g.,

D L1 1 BIB ABS

[36]There is also a file called CAOLD that has some papers earlier than 1967.

[37]For a discussion of *CA* online, see Ref. 15.

[38]There 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.

[39]Most commands can be used in three ways, as shown here. When the full term is spelled out (SEARCH), the system assumes an unsophisticated user, and gives more help. If the command is S, the system assumes the user is knowledegable about the system.

L1 means we are asking the system to display material pertaining to semipinacol, which is on line L1. If we fail to insert this information, the system will display items pertaining to the last L number shown.

1 means we are asking for information on the first of the four papers. The papers are listed in reverse chronological order, meaning paper 1 will be the latest of the four. Similarly, we can ask to see the information on any of the others.

BIB ABS means we are asking for bibliographic data (abstract number, title of paper, authors' names, journal, year, etc.) and for a display of the full abstract.[40] There are other choices. Instead of BIB ABS we could have typed CAN which would give us the abstract number only (we might then choose to find the other information in the printed *CA*). Or, we could have typed IND, which would give us the abstract number and the index terms for this paper, or ALL which would give everything we get from BIB ABS plus the index terms. In all, there are nine or ten ways to ask for display material. Our choice will depend on how much we need to know, and on the cost, since the more information requested, the higher the cost.

As so far described, online searching is faster then searching the printed *CA*, but gives us essentially the same information. The scope of the online method is much greater than that, for it allows us to combine words, in a number of ways. One such way is by the use of the terms AND, NOT, and OR. If we search AMBIDENT AND NUCLEOPHILE, we will get something like this:

332 AMBIDENT
3275 NUCLEOPHILE
L2 42 AMBIDENT AND NUCLEOPHILE

This means there are 42 entries that have the words AMBIDENT and NUCLEOPHILE somewhere in them; in the titles, keywords, or index entries. We can now, if we wish, display any or all of them. But a particular entry might have these two words in unrelated contexts, e.g., it might be a paper about ambident electrophiles, but which also has NUCLEOPHILE as an index term. We would presumably get fewer papers, but with a higher percentage of relevent ones, if we could ask for AMBIDENT NUCLEOPHILE, and in fact, the system does allow this. If we type S AMBIDENT(W)NUCLEOPHILE, we will get only those papers in which the term NUCLEOPHILE directly follows AMBIDENT, with no words in between.[41] This is called proximity searching, and there are other, similar commands. For example, the use of (4A) instead of (W) will give all instances in which the two words appear 4 or fewer words apart, in either order.

Another important option is a truncation symbol. If we ask for NUCLEOPHILE we will find all entries that contain the term nucleophile, but not those that contain a different form of this term, e.g., nucleophilic. We can take care of this by using NUCLEOPHIL? as a search term instead of NUCLEOPHILE. This will retrieve all terms that start with the letters NUCLEOPHIL, no matter what other letters follow, thus retrieving nucleophilic, nucleophilicity, nucleophiles, etc., as well as nucleophile. The question mark is one of several truncation symbols, each of which serves a different function.

The words AND, NOT, and OR are called *Boolean operators*.They may be combined in many ways, e.g.,

S ORTHO AND EFFECT AND HAMMETT

S (CARBON(W)DIOXIDE OR CARBON(W)DISULFIDE) AND CATALY? NOT ACID

S HYDANTOIN AND (METHYL OR ETHYL) NOT (VINYL? OR PHENYL)

[40]For some papers in the late 1960s only the bibliographic data, and not the abstracts, are available online.

[41]If we ask for AMBIDENT NUCLEOPHILE without the (W), the system treats it as if we asked for AMBIDENT(W)NUCLEOPHILE, and gives the same answers.

A particular search command can contain dozens of such terms. Obviously, if one is careful about choosing the proper search terms, one can focus in on just the relevent papers, and leave out those that will not be useful. However, there will often be far more papers than can conveniently be handled, and there are other ways to limit searches. One such way is by using a narrow field. For example, a synthetic chemist may wish to find references in which a given compound is synthesized, but find, when he or she searches for that compound, that most of the references concern biological or medicinal uses of the compound. By using the command

SEA 3489-26-7/ORG

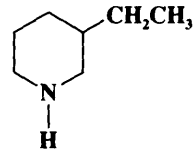
the search will retrieve only those papers for the compound of Registry Number 3489-26-7 that have been abstracted in the organic (ORG) sections of *CA* (Sections 21 to 34), and will not retrieve papers from the biochemical sections, which are more likely to stress biological or medicinal uses. There are many other ways to limit searches. It is possible to search only for papers in a single section of *CA*, only those that appeared in a given year or range of years, only those in which the search term appears in the title of the paper, only those by a given author, etc.

Besides subject terms, the CA File also contains bibliographical information, such as author names, location of the laboratory in which the work was done, language of the paper, etc., and these can be searched. For example, S ROBERTS, J?/AU will find all papers published by any authors named Roberts whose first name begins with J. These terms can be combined with subject terms in Boolean searches.

The Registry File

The Registry File is entered with the command FILE REGISTRY. This can be done at any time, and it is possible to go back and forth between the CA and Registry Files at will. The Registry File uses the same commands (including Boolean) as the CA File, but instead of displaying abstracts and bibliographical information, it displays information about compounds. Its most useful feature is that it allows the user to build a structure, and then gives information about compounds that possess that structure, even if the structure is only part of a larger structure (see below).

The procedure for building a structure can be long and complex, if the structure is large and complex, but the commands are simple. We will illustrate by building the structure for 3-ethylpiperidine, which uses the most important commands. We begin with the command



3-Ethylpiperidine

STRUCTURE. The system will ask if we wish to build on a structure previously used. If we say no, we will then get the prompt

ENTER (DIS), GRA, NOD, BON OR ?:

GRA is used for putting in chains or rings. We enter GRA R6, DIS (the DIS must be typed if the structure is to be displayed), and get the structure **1** shown in Figure A.1.[42] R6 specifies

[42]The structures shown in Figure A.1 are those received by ordinary computer terminals. Better-looking structures, more like those printed in books, are obtained with certain types of terminals. The system always asks the user to specify which type of terminal is being used.

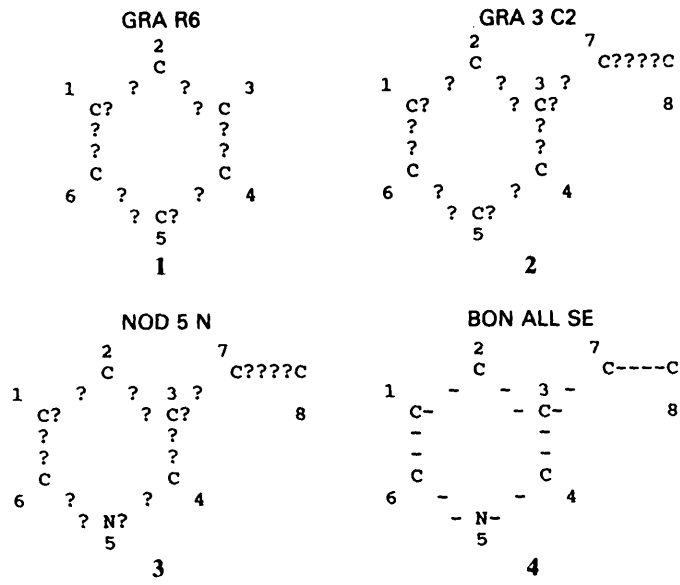


FIGURE A.1 Steps in building the structure of 3-ethylpiperidine in the Registry File. Above each structure is the command that gave that structure.

a 6-membered ring. If we had simply entered 6 we would have created a six-atom chain. The six numbers shown are purely arbitrary and have no connection with the way the positions are actually numbered in any nomenclature scheme. Immediately after this structure is displayed, the same prompt reappears, as it does after every structure. We wish to introduce a two-atom side chain (the ethyl group), so we enter GRA 3 C2, DIS, and get structure **2** in Figure A.1. The C2 indicates a two-atom chain, and the 3 means that we want it attached to atom 3 (in this case the atom number is completely arbitrary, since attachment to any atom would give an equivalent result). Note that the system has numbered the new atoms 7 and 8. We will not be introducing any more atoms into our structure, but if we were they would be numbered consecutively, in the order in which they were introduced. We have all the atoms we need (we do not indicate the hydrogens because the system assumes that all nonspecified valences are connected to hydrogen, unless we tell it otherwise), but we still have not told the system about the nitrogen. Although the system uses C to specify all atoms, they will only remain carbon atoms until we instruct the system differently. To get 3-ethylpiperidine the atom in the 5 position must be nitrogen. A C can be changed to another element by using NOD (for node), so we now type NOD 5 N, DIS. This changes C-5 to N-5, giving all the atoms in their final positions (**3** in Figure A.1). However, the structure is still not complete because the bonds have not been specified. By using the BON command we can make any bond single, double, or triple, and can even indicate aromaticity or other resonance. In this case we want all the bonds to be single bonds, so we type BON ALL SE, DIS (SE is used for single bonds), and get our final structure **4** in Figure A.1.

At this point we type END, and get

L1 STRUCTURE CREATED

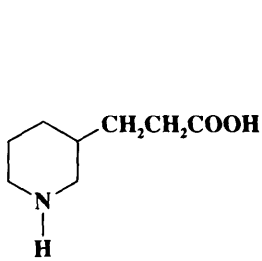
The structure is now ready to be searched. At the command SEARCH L1, the system will give the prompts

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:

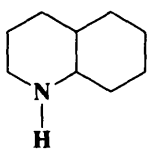
The system asks for the desired scope, because a full search (of the entire Registry File of more than 10 million substances) may cost a lot of money and may not be worth it if the desired answers can be obtained from a more limited search.

As shown by the first prompt there are four types of search, of which we will discuss two: exact and substructure (SSS). In an exact search, only information regarding exactly the structure given will be retrieved, but even so there may well be several answers, because *CA* treats stereoisomers and isotopically-substituted compounds as separate answers. At the conclusion of the search the system gives the number of answers, e.g., 4. We may now look at the four answers by using the display command. As in the CA File, there is a choice of display formats, but if we choose SUB we will get (1) the Registry Number, (2) the approved *CA* index name, (3) other names that have appeared in *CA* for that compound, (4) a structural formula, and (5) the number of *CA* references since 1967, along with a notation as to whether the compound is found in the CAOLD File. By using other display formats, we can also obtain the bibliographic information and abstracts for the latest 10 references. If there are more than 10 *CA* references, we can of course switch to the CA File, and use the Registry Number to search that file completely. If the exact structure search yields no answers, we know that no references to it have appeared in *CA* since 1967.

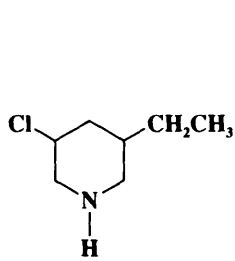
Although an exact search can be useful, in most cases it does not give any more information than can be obtained from the printed *CA*. Substructure searches (SSS) are far more important, because there is no other way to get this information. If we do a substructure search on **4** in Figure A.1, we not only get all the answers we would get in an an exact search, but all substances that contain, anywhere within their structure, the arrangement of atoms and bonds shown in **4.** For example, **5, 6, 7,** and **8** would all be retrieved in this



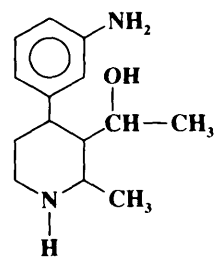
5



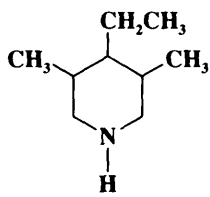
6



7



8



9

search, but **9** would not be. SSS searches typically retrieve from tens to hundreds of times as many answers as exact searches of the same structure. Furthermore, the scope can be widened by the use of variable nodes. For example, the symbol X means any halogen, the symbol M any metal, and the symbol G allows the user to specify his or her own variable at that point (e.g., G = Cl or NO_2 or Ph). As with an exact search, each answer can be displayed as described above.

As mentioned above, building structures can be very complicated, and, because there is great flexibility in the system, there are a great many ways to use the commands, but the

rewards are the retrieval of information that cannot be obtained in any other way. We have given here only a hint of the possibilities in using this system.

It is not necessary to build structures to use the Registry File. Compounds can also be searched for by using names, combinations of name fragments, Registry Numbers, molecular formulas, and in other ways. The display methods are the same.

Other Databases

Several of the other databases carried by STN are of interest to organic chemists. Among these are BEILSTEIN, which allows Beilstein to be searched online (SSS and EXACT searches can also be done in this database); CASREACTS, in which the user can specify a starting compound and a product, usually by giving Registry Numbers, and the system tells whether that transformation has been reported in the literature (beginning in 1985), and if so gives reagents and references; and CJACS, which gives the complete texts (but not the display material, such as tables and displayed equations) of all papers published in about 20 journals published by the American Chemical Society (including *J. Am. Chem. Soc.*, *J. Org. Chem.*, and *Chem. Rev.*) since 1982. Chemical journals of several other publishers, including Elsevier (*J. Organomet. Chem.* etc.), VCH (*Angew. Chem. Int. Ed. Engl.*), and the Royal Society of Chemistry (*J. Chem. Soc., Perkin Trans. 1* etc.), are also available online in a similar manner. Having these journals online is particularly useful because their texts can be seached for keywords, author's names, Registry Numbers, and other types of information.

Science Citation Index

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, etc. But for obvious reasons the paper itself supplies no way to locate *later* papers. *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 43901 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 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.

SCI covers about 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 two-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*[43] *Subject Index*. This index alphabetically lists every significant word in the titles of 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 co-word. The user is then led to the *Source Index*, where the full reference is given. *SCI* is also available online (though not through STN) and on CD-ROM discs. 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 about 2500 journals in the same general areas as are covered by *SCI*. The review articles cited appeared in about 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.

How to Locate Journal Articles

Having obtained a reference from Beilstein, *SCI*, *CA*, a treatise, or some other source, one often needs to consult the original journal (the location of patents is discussed on p. 1243). 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.*, *Chem. Ber.*, etc., 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)*, 1989 edition, which contains the names of all the journals covered by *CA* from 1907 to 1989 (even those no longer published), with the most recent abbreviations in bold print. 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

[43]Registered trade name.

student will find that usages vary from country to country, and even from journal to journal within a country. Futhermore, the *CA* abbreviations have changed from time to time.

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.A. Orders for documents can be placed by mail, telephone, Telex, fax, or online through STN or other services.