

Organic Synthesis

Finding Procedures and Methods in Synthetic and Reaction Chemistry

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SELECTED REFERENCE SOURCES NO. 113
DAVID FLAXBART, COMPILER

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I. OVERVIEW

A question about a synthesis or a reaction can be approached from a number of different angles, some of which are straightforward, and others of which require more time and effort. The simplest approach is finding a preparation for a known organic substance. Other aspects, such as starting materials, reaction types, mechanisms and sites, conditions, yields, catalysts, and functional groups, can be more difficult to locate quickly.

The literature of organic chemistry is vast and extends far back in time. The bulk of the *primary* research literature is from journals, but in recent years patents have provided another major source of preparation information. Later, this information may be republished in the *secondary* literature, which includes handbooks, compendia, indexes, reviews, textbooks, and treatises.

If you're starting from scratch, consulting the secondary sources can greatly reduce time spent searching the literature. This guide aims to describe the most useful and best-known of these, and act as a guide to finding preparation and reaction information in the Chemistry Library. Sources listed are located in the reference collection unless otherwise noted, but it's always a good idea to check UTCAT for the current location and status of any book you're seeking.

While organic chemistry is a rapidly developing and expanding field, its literature has a relatively long "half life" compared to some other chemical disciplines. This makes the concept of *retrospectivity* important.

II. FIRST-STOP SOURCES: Chemical "Dictionaries"

Finding relevant names, synonyms, formulas, and CAS registry numbers should always be the first step, and having this data up front will save time in the long run. Many of the basic handbooks in chemistry provide useful information to point you in the right direction, particularly in identifying and naming a compound—whether it's the desired product, a starting material, reagent, catalyst, or whatever. Some basic handbooks and catalogs also provide a shortcut to synthetic methods found in other handbooks, such as Beilstein, and provide CAS registry numbers as well. The following are listed in basic order of first look.

CRC Handbook of Chemistry and Physics.

Handbook Table

Each edition of the CRC contains a table of physical constants for organic compounds, giving mol. wt., color, bp, mp, density, solubility, and a Beilstein reference. Consult the table's own indexes as well as the index in the back of the volume. A ring structure section, formula and synonym indexes follow the table.

CRC's nomenclature can be puzzling, but a substance is usually found under the common parent name. Published annually.

Aldrich Catalog Handbook of Fine Chemicals.

Handbook Table

Multi-use catalog of the Aldrich Chemical Co., listing over 27,000 chemical products. The Aldrich is particularly useful as a starting point because entries include molecular and structural formulas, basic physical data, and cross-references to Beilstein, Merck, Aldrich's spectra and safety collections, and Fieser's *Reagents for Organic Synthesis*. Also available on the CD-ROM workstation.

Merck Index. (12th ed., Merck, 1996)

Handbook Table

Descriptions of over 10,000 chemicals, drugs, and biological substances. Entries include name, synonyms and trademarks, formula, molecular weight, structure, some physical data, and remarks on nature, occurrence and uses. Indexed by synonym, CAS registry number, therapeutic category and biological activity, and formula. The text of the Merck "monograph" (i.e. entry) often includes one or more literature references for preparation methods, including patents.

Dictionary of Organic Compounds. (Heilbron) (6th ed., Chapman & Hall, 1994)

Handbook Table 7 vols., with supplements and indexes

Entries are alphabetical by name, and contain physical data, structure, CAS registry number, and often references to preparation literature (designated "synth"). Covers about 150,000 compounds; derivatives are listed with the parent. Indexes in vols. 6 and 7 contain compound listings for the base set by name/synonym, molecular formula, heteroatom, and CAS registry number.

Handbook of Data on Organic Compounds. (HODOC) (3rd ed., CRC, 1994)

Handbook Table 7 vols.

Data collection, giving names, synonyms, structures, formulas (line and molecular), physical constants, solubilities, spectral data (IR, Raman, NMR, UV, Mass), as well as CAS registry numbers and Beilstein references. Does not contain literature references or preparation information. Index volumes: vol. 7 – synonyms, vols. 8-9 – formula, mp, bp, mw, plus extensive spectral data indexes. Also available on CD-ROM as "Properties of Organic Compounds."

Dictionary of Organometallic Compounds. (Chapman & Hall, 1984)

QD 411 D53 1984 3 vols., plus supplements

Sections arranged by metal element, and sub-arranged by molecular formula in Hill order. Entries give CA index name and synonyms, structure diagram, Registry Number, mol. wt., physical and toxicity data where available, and literature references. Vol. 3 has indexes for name, molecular formula, and registry number.

Reagent Chemicals. (8th ed., ACS, 1993)

QD 77 A54 1993

Official ACS specifications for standard reagents.

III. BASIC SYNTHESIS COMPENDIA

These are usually the smaller collections of methods, in English and with good indexing.

Organic Syntheses. (Wiley, 1921-)

QD 262 O7 and QD 262 O722 (Collective Volumes)

Annual compilations of checked laboratory methods. The procedures in this series contain enough detail to make going to the original literature unnecessary in most cases. Emphasis is on model compounds and important reaction types.

The annual volumes are periodically revised and reissued as the **Collective Volumes**. The latest **Cumulative Index** covers Collective vols. 1-8 and contains nine separate indexes: name and CA name, reaction type, compound type, formula, solvents and reagents, apparatus, author, and general subject/name. If you have a citation to the original OS entry, translate this to a Collective page number by checking the concordances in the back of the appropriate collective volume.

The **Reaction Guide** (1991) summarizes in structural diagram format all procedures published in the series through Collective vol. 7 and annual vol. 68, and gives the OS citation. Reactions are classified into one of eleven types.

New annual volumes are shelved in Reference until superseded by a Collective Volume. Older OS are shelved in the stacks.

Compendium of Organic Synthetic Methods. (Wiley, 1971-)
QD 262 C53

Systematic listing of functional group transformations, classified by functional group of starting material and product. See introduction for use instructions; not a cumulative set.

Survey of Organic Syntheses. (Wiley, 1970)
QD 262 B78 2 vols.

Chapters discuss functional groups and give brief synthetic procedures. With subject and author indexes; cumulative reaction index in vol. 2.

Purification of Laboratory Chemicals. (Perrin) (4th ed., Butterworth-Heinemann, 1996)
TP 156 P83 P47 1996

Not a collection of syntheses, but a useful guide to methods for purifying common reagents. Chapters describe basic physical and chemical techniques, then list about 4,000 organic compounds, 750 inorganics and metal-organics, plus some biological chemicals. Entries state with varying length the best technique(s) to use.

The Chemical Formulary. (Bennett) (Chemical Publishing, 1933-)
TP 151 B35

This series acts as a handy "cookbook" for the preparation of common home and industrial products, ranging from soaps to varnish removers and the like. There is a cumulative index for vols. 1-25.

IV. THE HANDBUCH: Beilstein and Houben-Weyl

Every organic chemist should be acquainted with these large handbook series. As with smaller sources, these tools draw their information systematically from the primary journal literature, checking and summarizing methods and techniques reported. They can also be somewhat intimidating, especially for a novice, because of their size, complex arrangements, and German language.

Beilstein's Handbook of Organic Chemistry. (4th ed., Springer, 1918-)

Reference Stacks

Indexes on Beilstein Index Table

The most extensive source for property and synthesis information on carbon compounds. Access is either through the Indexes (formula and name) or by the "Beilstein System" of compound classification. The Basic Work (Hauptwerk) and its first four Supplements (Erganzungswerke) cover the organic literature comprehensively and critically up to 1959. The 5th Supplement covers heterocyclic compounds between 1960 and 1979. (The Library stopped buying new volumes in 1990.) See user guides on the Index Table for further information.

Finding a compound in Beilstein can be easy if that compound is listed in the CRC, Aldrich Catalog, Lange's Handbook, or the HODOC. All of these tools provide Beilstein citations. Once you know the Beilstein volume number for your compound, you can consult the formula index for that volume (on Index Table) to retrieve page numbers for all five sections indexed (H, EI-EIV). Remember that the

compound's System Number and volume number do not change over time, and you can trace it backward and forward through the Supplements by noting these numbers.

The Beilstein System classifies organic compounds by chemical structure; all substances containing metals are excluded by definition. The arrangement is summarized:

Volumes 1-4 Acyclic (no rings)
Volumes 5-16 Isocyclic (carbon-only rings)
Volumes 17-27 Heterocyclic

Beilstein entries include references to formation (Bildung or B.) or preparation (Darstellung). Entries will give starting materials, but rarely enough detail about the procedure to recreate it without consulting the original document. This giant German series is most useful if you're searching for synthesis or reaction information for specific substances; it's less useful if you're seeking details on reaction types or conditions, byproducts, yields, reagents, catalysts, or functional groups. **This type of information is more accessible via Beilstein's Crossfire system (see below).**

Methoden der Organischen Chemie. (Houben-Weyl) (4th ed., Thieme, 1952-)

Reference Stacks QD 258 M44

Extensive German series giving selected and detailed laboratory methods for preparation of organic and organometallic compounds, along with some macromolecules and specific functional groups. Experimental conditions are detailed enough to allow reproducing a synthesis without consulting the original document. Each volume and its subparts discusses specific classes of compounds. HW is structured according to the type of product formed. Only the principal function is considered, as defined by the level of oxidation, substitution or saturation of the carbon atom(s). Transformations of the principal functional group are illustrated by typical examples, presented as a methodological overview with extensive references.

The basic volume arrangement can be summarized broadly:

I - IV: General chemical and physical methods
V - XIII: Chemistry of Compound Classes
XIV: Macromolecules
XV: Peptide Synthesis
XVI: Indexes
E1- Supplemental Volumes

Subject indexes in the subvolumes give German chemical names; there are also detailed tables of contents. The three parts of vol. 16 are indexes for vols. 1-15 and supplements E1-E5 and E11 (i.e. to 1985). Vol. 16/1 is an index of 800 compound classes (by German name) and 100,000 single compounds (by formula). Vol. 16/2a lists 240 acyclic classes and 20,000 subclasses, arranged systematically. Vol. 16/2b is an index of cyclic compounds by ring size.

The easiest approach to the series is to select the volume dealing with the compound class or functional group in question and consult its table of contents; relatively few of the many compounds discussed actually appear in the "cumulative" indexes. The quality and scope of individual volume indexes vary widely, and they should be used cautiously.

H-W was published in German until 1990, but a good German chemical dictionary will help.

V. REACTION CHEMISTRY SOURCES

The following tools are basically more reaction-oriented than substance-oriented and are good to consult if you're interested in mechanisms and processes rather than "recipes."

Comprehensive Organic Transformations. (Larock) (VCH, 1989)

QD 262 L355 1989

Condensed, systematic compilation of useful synthetic methodologies. Reactions are organized by functional group being synthesized, and subdivided by major processes. Transformation index in the back.

Organic Reactions. (Wiley, 1942-)

QD 258 O7

This series concentrates on name reactions and other well-known types. Each volume is a collection of several chapters, each devoted to a single reaction or phase. Emphasis is on preparation, giving detailed procedures for each method, plus examples and bibliographies. Tabular surveys relate the molecular environment to the appropriateness of using a particular reaction; compounds listed in these tables are not found in the indexes. Cumulative topic chapter indexes appear in each volume; likewise there are author indexes.

Theilheimer's Synthetic Methods of Organic Chemistry. (Karger, 1940-)

QD 262 S9675

Annual (now semiannual) compendium of synthetic reaction information drawn from a cognate publication, the *Journal of Synthetic Methods* (not held at UT), and from the non-patent literature. Theilheimer is reaction-based, and reactions are selected carefully according to predefined criteria; only general reaction types are included, and most heterocyclic chemistry is omitted. Reactions must have high yield and give full experimental procedures. Reactions must meet one or more of these criteria:

- novel reactions, methods or reagents of synthetic interest
- significant modifications or interesting applications of known reactions
- reviews

Reactions are classified according to 1) bond formed, 2) reaction type, and 3) bond broken, in that order. Each volume has a subject index listing classes of compounds as either starting materials or products, and these are cumulated at five-year intervals. Name reactions and reaction types are usually avoided. Each volume also includes a listing of Supplementary References showing modifications or improvements to reactions listed in earlier volumes. Lastly, each volume's introduction is a useful review article highlighting developments in the field during the year in question.

Theilheimer's selectivity and arrangement make it more useful as a browsing tool to keep current with developments in the field; it's less valuable as a source of specific preparation methods.

For definitions and schemes of well-known name reactions (i.e. reactions named for the chemists who devised the technique), you should also consult the following dictionaries:

Name Reactions and Reagents in Organic Synthesis. (Wiley, 1988)

QD 291 M86 1988

Useful compilation of name reaction data, giving general scheme, mechanism, examples, and references. Reagent section lists uses, preparation, examples, and references.

Name Reactions in Organic Chemistry. (Academic, 1961)

QD 291 S8 1961

Descriptions of about 70 name reactions in alphabetical order. Subject index in back excludes these names; consult table of contents for them.

Named Organic Reactions. (Wiley, 1998)

QD 291 L35 1998

Organic Name Reactions. (Wiley, 1964)

QD 291 K713 1964

Alphabetical listing, giving diagrams and many references.

VI. USEFUL TREATISES

Occasionally it's more useful to consult an encyclopedia-type text rather than a list or index of particular methods or reactions. These offer a more general and logical introduction to various topics than a series or index can. A number of these are excellent starting points for learning about reactions and chemical mechanisms for particular types of compounds, and they contain numerous literature references.

Comprehensive Organic Chemistry. (Pergamon, 1979)

QD 245 C65 6 vols.

All classes of organic compounds are represented. Vols. 1-3 cover various functional groups, vol. 4, heterocyclics, and vol. 5, biological compounds. Vol. 6 is a series of indexes by formula, reagent, reaction, subject, and author. Many literature references are also included.

Comprehensive Organic Functional Group Transformations. (Pergamon, 1995)

QD 262 C534 1995 7 vols.

Massive attempt to organize current knowledge of organic synthesis in terms of the introduction and interconversion of functional groups. Volumes are broken down by the number of attached heteroatoms. Subject and author indexes are in v. 7.

Comprehensive Organic Synthesis. (Pergamon, 1991)

QD 262 C535 1991 9 vols.

Each volume of this set deals with a particular type of reaction or bond formation and has its own author and subject index. Articles are comprehensive reviews written by recognized experts. Vols. 1 and 2 cover additions to C-X pi-bonds; vol. 3, C-C sigma-bond formation; vol. 4, additions to and substitutions at C-C pi-bonds; vol. 5, combining C-C pi-bonds; vol. 6, heteroatom manipulation; vol. 7, oxidation; vol. 8, reduction; and vol. 9, cumulative author and subject indexes. A good reference tool for both specialists and occasional users.

Comprehensive Heterocyclic Chemistry. (Pergamon, 1984)

QD 400 C65 1984 8 vols.

Covers compounds with rings that have at least one non-carbon atom. Chapters are arranged by ring type and discuss structure, reactivity, and synthesis. Volume 8 has indexes by subject, author, ring system, and physical data values. In 1996 *Comprehensive Heterocyclic Chemistry II*, an 11-volume "sequel," appeared, updating the literature coverage.

Comprehensive Coordination Chemistry. (Pergamon, 1987)

QD 474 C65 1987 7 vols.

Overview of the field, surveying binding of ligands, coordination chemistry of the elements in Periodic order, and applications. Indexes by subject and formula are in vol. 7. This set complements *Comprehensive Organometallic Chemistry*, and the division between them is somewhat arbitrary.

Comprehensive Organometallic Chemistry. (Pergamon, 1982)

QD 411 C65 1982 9 vols.

Compilation of current organometallic and carbon monoxide chemistry, reviewing the elements individually, surveying uses in synthesis and catalysis, bonding, behavior in solution, and environmental impact. Vol. 9 has indexes by subject, author, formula, and structure type. Use in conjunction with the above set. In 1995 *Comprehensive Organometallic Chemistry II* appeared, updating the original set.

Encyclopedia of Reagents for Organic Synthesis. (Wiley, 1995)

QD 262 E53 1995 8 vols.

Extensive entries for 3000 reagents, containing physical data, solubility, preparative methods, uses, and descriptions. Entries are arranged according to IUPAC names. Indexes in v. 8 allow searching by reaction type, name reactions, substrates, formulas, structural class, and reagent function.

Reagents for Organic Synthesis. (Fieser & Fieser) (Wiley, 1967-)

QD 262 F5

Popular compendium of uses of common and new reagents including preferred methods of preparation, supply sources, critical comments, reaction diagrams and structural formulas, and many literature references. Arranged alphabetically with subject, author, and reagent indexes in each volume. There is a cumulative index for vols. 1-12. The Aldrich Catalog denotes "Fieser" references for many compounds and acts as a shortcut index.

Rodd's Chemistry of Carbon Compounds. (2nd ed., Elsevier, 1964-)

QD 251 R6 1964

Arranged in multi-part volumes with supplements:

- I - Aliphatic (chain)
- II - Alicyclic
- III - Aromatic
- IV - Heterocyclic

Each volume or supplement is essentially a stand-alone monograph on the chemistry of specific types of compounds, with its own index. Types of compounds in each volume are listed on the spine. There is as yet no cumulative index.

Advanced Organic Chemistry: Reactions, Mechanisms, and Structure.

(4th ed., Wiley, 1992)

QD 251.2 M37 1992 (Reserves)

March's classic text on all aspects of the field, with emphasis on bonding and reactions. Plus a useful survey of the literature of organic chemistry in the last chapter.

Handbook of Organic Chemistry. (Prentice-Hall, 1996)

QD 251.2 B4813 1996

Translation of the classic German treatise *Lehrbuch der Organischen Chemie*, 22nd edition. Handy one-volume compendium.

Chemistry of Functional Groups. (Patai) (Wiley, 1964-)

Stacks (see UTCAT for call numbers of individual volumes)

Respected series of books dealing with the characteristics, synthesis, and chemical nature of particular classes of compounds. For a complete guide and index to the series, see *Patai's 1992 Guide to the Chemistry of Functional Groups*, in reference at QD 251.2 P34 1992. This volume is annotated showing call numbers of the individual volumes in the collection. Check UTCAT for up-to-date status and location information. (The library does not own all volumes.)

Chemistry of Heterocyclic Compounds. (Wiley, 1950-)

Book Stacks QD 399 C534

Series of volumes of original articles and reviews dealing with the syntheses, reactions, properties, structures, physical chemistry, and utility of compounds belonging to specific ring systems or classes. Each volume deals with a specific compound type and has a separate record in UTCAT. There is no series index.

A Guide for the Perplexed Organic Experimentalist. (2nd ed., Wiley, 1990)

QD 261 L63 1990

This little primer offers an informative, informal overview of the problems a neophyte might encounter. Its first chapter is a guide to the printed literature and reference sources; chapter 2 discusses online information retrieval. Other chapters deal with laboratory issues such as purification, safety, and basic techniques.

VII. NOMENCLATURE AND TERMINOLOGY

Written language has long proven inadequate to the task of expressing the precise structure and composition of a molecule, despite the best efforts of IUPAC and other groups to establish standard rules. The only unambiguous way to depict a substance is with a structural formula diagram. The name you use for a particular substance will vary according to the source you're looking in: CA, CRC, Beilstein, etc. all use different systems of nomenclature, greatly adding to the confusion. For this reason having a registry number or a molecular formula up front will be a good head start.

If you need a brief definition of a class of compounds, or help naming a compound correctly, consult some of the following for help. Many other general dictionaries of chemistry are in reference at QD 5.

Concise Etymological Dictionary of Chemistry. (Applied Science, 1976)

QD 5 B57

Very useful source of definitions for prefixes, suffixes, and other parts of chemical terminology, and their origins.

Desk Reference for Organic Chemists. (Chapman & Hall, 1995)

QD 257.7 E28 1995

Definitions of chemical and physical acronyms, stereochemical and synthetic terms, name reactions and reagents, with a useful listing of review references.

Hawley's Condensed Chemical Dictionary. (13th ed., Van Nostrand, 1997)

QD 5 C5 1997

The best all-around dictionary of chemistry, strong on defining classes of compounds, functional groups, important substances, techniques, equipment, etc.

Naming and Indexing of Chemical Substances for Chemical Abstracts.

CA Index Guide, Appendix IV (CA Index Table)

More than you'd ever want to know about how CA selects names for compounds it indexes.

Nomenclature of Organic Chemistry. (Pergamon, 1979)

QD 291 I57 1979

IUPAC's "blue book" of collected recommendations on nomenclature of hydrocarbons, heterocyclic systems, and others, plus sections on stereochemistry, natural products, and isotopically modified compounds.

The Vocabulary of Organic Chemistry. (Wiley, 1980)

QD 291 C55 1980

Not a typical dictionary, but a series of chapters grouping organic concepts and defining terms, with examples. Consult the index and table of contents.

VIII. REVIEWS, SURVEYS, AND ABSTRACTING SERIALS

There are a number of publications—annuals, review journals, and abstract services—that take a broad look at the enormous literature of this field and help chemists stay up to date with recent developments. Some have already been listed above (e.g. *Organic Reactions*, *Theilheimer's*, etc.) Here is a brief selection of others:

Annual Reports in Organic Synthesis. (Academic, 1970-)

Book Stacks QD 262 A558

Abstracting service covering about 50 of the most relevant journals. Entries consist mainly of structure and reaction diagrams. No subject index, so consult the table of contents. Author index lists first author only.

Chemical Reviews. (ACS, 1924-)

Journal Stacks by title

Major ACS journal that publishes review articles in all chemical fields.

General and Synthetic Methods. (RSC, 1976-93)

Book Stacks QD 262 G45

Annual literature review published by the Royal Society of Chemistry. Coverage ran about three years behind (e.g. the volume published in 1993 covers 1990). Mutated into the review journal *Contemporary Organic Synthesis* in 1994, which was in turn absorbed into *J. Chem. Soc. Perkin. I* in 1998.

Methods in Organic Synthesis. (RSC, 1984-)

Journal Stacks by title

Monthly current awareness journal published by the Royal Society of Chemistry. Each issue is indexed by reactant, reagent, product, and reaction. Reaction diagrams include yields and other information.

Coverage of organic journals is selective and emphasizes rapid communications of novel experiments.

Natural Product Reports. (RSC, 1984-)

Journal Stacks by title

Bimonthly journal covering developments in bioorganic chemistry and the separation and biosynthesis of natural products.

Organic Reaction Mechanisms. (Wiley, 1965-)

Book Stacks QD 258 O82

Annual review volumes; excludes reaction topics in electrochemistry, photochemistry, organometallics, surface chemistry, and heterogeneous catalysis.

There are a number of other review publications both narrowly and broadly defined; consult a guide to the literature to find useful titles. Other research journals often publish reviews along with primary research results. *Chemical Abstracts'* printed indexes indicate a review paper with the prefix **R** in the abstract number. Online, search the keyword "review" in the abstract text to find them in context with a topical search query.

IX. DIGITAL SOURCES

Online searching allows you to be much more specific when seeking information on syntheses: you can specify more variables, such as starting products, conditions, yields, and other parameters in some files, and limit results quickly by date, language, format, etc.

BEILSTEIN CROSSFIRE plus REACTIONS

The online version of this giant resource allows much more powerful searching for preparative information than can be done in the printed handbook. The online file also allows structure searching: you can do a substructure search to gather compound or reaction records of interest.

Unlike bibliographic files such as CA, Beilstein is retrospective and contains all compound information found in the printed handbook as well as more current unchecked information gathered from a large number of publications and patents. It contains records for over 7 million carbon compounds and 7 million reactions, and is second only to CAS Registry in size and scope. It is updated quarterly.

Beilstein Crossfire is available on workstations in the Chemistry Library, and the client software is distributed free to UT-affiliated persons who would like to load it on their own machines. A site license for the system makes searching it free of charge for UT users. Consult the library's web page or available documentation for further information:

<http://www.lib.utexas.edu/Libs/Chem/xfire.html>

CA Online

Chemical Abstracts online goes back to 1967. The full file with abstracts is available on the STN network, on Dialog (without abstract text), and a number of other commercial vendors. The Student Edition, which includes records from 250 major journals, is available on the worldwide web through UT Library Online.

Finding preparation information for specific compounds in CA is easy: search the registry number with the suffix P:

STN: s 9878-98-4p
Dialog: s rn=9878-98-4p

CA appends a P to all registry numbers in a record for which some preparation information is given in the document being indexed. This does not guarantee that this information is extensive or detailed, only that some preparation information is there. When a non-specific derivative of a registered compound is described, CAS appends a D to the registry number in the CA file.

When searching abstract or indexing text, be sure to use the abbreviation "prepn" as well as the spelled-out word when linking to other keywords or registry numbers. Remember that searching generic terms like "synthesis" and "reaction," especially in truncated form, can slow the system down considerably or exceed retrieval limits since so many records contain these words. Always be as specific as possible.

Registry

This giant file of over 17 million compound records (the vast majority organic) complements CA and is the source of registry numbers for searching in CA and other online files, as well as many printed works. It is the site of name, synonym, name part, molecular formula, ring data, and structure for compounds registered by CAS—data elements that are NOT duplicated or searchable in the CA file. The file may be searched by "dictionary" term (such as molecular formula, ring data, name fragment, etc.) or by drawing a structure. Substructures can be searched to identify a set of compounds sharing a common structural component. Results can then be crossed over to the CA file where the literature from 1967 can be searched quickly and efficiently.

Any completely described substance—product, reactant, or intermediate—that appears in a document indexed by CAS receives a registry number and is entered in the database. If a desired substance is not in the database, as determined by several searches, including exact structure, you can be reasonably certain that compound has not been described or mentioned in the literature since 1965. (Registry is not fully retrospective.) A substructure search to find similar compounds which might serve as models or starting points is the next step. Take the L-numbered set retrieved this way (not too many, hopefully), cross it over to the CA file, and search for preparation information on these registry numbers:

=> s L2/P

With luck some of the hits will result from articles discussing preparation of similar types of substances.

No actual chemical or preparation data is contained in Registry; it is simply a source for identification of a specific compound (including isomers and derivatives) or group of compounds which can then be searched in other databases. The full Registry file is available only on STN. Searching by chemical structure is best done using a graphical drawing/communications program called STN Express.

CASREACT

CASREACT contains information on 1.2 million single-step and 1.7 million multistep organic reactions, drawn from *Chemical Abstracts'* organic sections since 1985. Information includes reactants, solvents, and catalysts. The file is searchable by structure of reactants, functional group codes, registry numbers, yields, bibliographic data, substance and subject indexing terms, and CA abstract numbers. This file is available only on STN.

SCIENCE CITATION INDEX

This database allows you to look forward in time by indexing citations to earlier papers. For instance, if you have an important paper that's quite old, you can find later papers that draw on its work. This is a completely different way of approaching the literature than a subject-based index like Chemical Abstracts, and it can be a very useful complement to other methods. SCI is available on the library's CD-ROM network in all library units. Consult the SCI handout for searching instructions.

UTCAT

The library's online catalog is a good place to search for **books** on broad topics in organic synthesis, particularly the chemistry of specific compound classes or functional groups, or well-known reaction mechanisms. It is *not* usually a good place to find information on specific compounds or narrow topics, however.

Search for established subject headings using the S command. For example:

s ketones
s friedel-crafts reaction
s chemistry, organic--synthesis
s heterocyclic compounds

Keyword searches are both more flexible and powerful since you can search in several fields in the records without being tied to predetermined Library of Congress headings. For example, the search

s friedel-crafts reaction
pulls up 11 records; the alternate search
tk friedel crafts

results in 15 hits. For this reason keyword searching is usually a better option.

X. CHEMICAL ABSTRACTS (Printed)

If you're searching comprehensively or if you're seeking preparation or reaction information on relatively new or obscure compounds, natural products, pharmaceuticals, complex molecules, or polymers, *Chemical Abstracts* is the best entry point into the literature. CA's coverage of chemical patents worldwide is unsurpassed, making it the tool of choice if you're seeking patented techniques or compounds. CA does have some limitations when dealing with reaction chemistry. Its indexing policies can exclude intermediates or techniques unless the source document defines them fully and presents some new information about them.

Patents are indicated in the CA indexes with the prefix **P** in front of the abstract number, in case you want to exclude them and save time. Review articles are similarly designated by an **R**. You have to look at the abstract itself to determine the language of the publication, however.

1. Common Compounds—Preparation

Check in the Index Guide for the literature period in question under a common name or abbreviation, and note the CA Index Name. Use the Index Name to search for entries on the compound in the Chemical Substance Indexes (Collective or Six-Month). Under the heading for the compound in this index, search for the entries by the keywords "prepn" or "reaction." A one-line summary of a document will appear with its abstract number. If your compound is one of 600 or so "Qualified Substances" (elements and common compounds very frequently cited), look for the boldface headings "**preparation**" and "**reactions**" which group entries on these topics. The "**preparation**" heading includes manufacture, synthesis, separation, and purification all together for ease of browsing. "**Reactions**" includes modifications, corrosion, isomerization, neutralization, etc.

2. New, Novel, or Obscure Compounds, Derivatives, Esters, Salts, etc.

If you have a systematic name, check both in the Index Guide and the Chemical Substance Index to see if the compound is listed as such. Frequently it will not be there because CA uses its own nomenclature rules that don't always exactly follow IUPAC standards. Derivatives are listed after the parent compound in this index, making browsing easier. Check the Index Guide to determine what CAS calls the parent. If you have a molecular formula, check the most recent collective Formula Index to locate an index name that might match your compound. Use this name to consult the Chemical Substance Index as described above. Parent names for ring compounds can be identified in the Ring Systems Handbook.

If you find nothing, an online search in the Registry database is probably the only other effective way to see if your substance has been identified in the literature and registered by CAS. See below for more details.

3. Reaction Types, Classes of Compounds, Techniques, Miscellaneous Topics

Always consult the Index Guide to find an appropriate heading to look under. CA's controlled vocabulary is very carefully selected, but is not always intuitive. Take this term to the General Subject Indexes (Collective or Six-Month) to find abstract numbers. CAS always assigns the most specific headings possible, so be sure to consider

your choice of terms carefully. Useful information about a more general topic may not be found if you search under very specific terms, and vice-versa.

It is not always easy to locate relevant publications on the fine points of reaction chemistry using printed *Chemical Abstracts* because of the rigidly controlled indexing vocabulary and coverage policies. It can also be quite time-consuming using the printed indexes. Online searching is a viable alternative, but first consulting some of the treatises listed above can get you into the older literature faster and give you more ideas about what terms or concepts to search for in CA. As always with an abstract source like CA, the more you know about your topic up front, the more likely you are to find useful information quickly.

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