

Data Collections

Just as libraries can be organized by subject classification (grouping books on the shelf by subject area) or by indexing (creating records describing the book - author, title, subjects, etc. - and indexing the various types of information), so too, the primary scientific literature can be organized in two broad ways: indexing, or selecting data from the published literature and bringing them together in collections. This lecture will look at the various forms of data collection.

These are a form of secondary literature in which an editor selects information from primary sources and arranges it to facilitate a particular type of access.

Often, the data are reviewed and evaluated by the editors before inclusion, adding further value.

The right data collection can be more useful than searching primary sources, depending on the objective of your search. If you're looking for a specific piece of data, or an introduction/overview of an area you are not yet expert in, data collections can save you a lot of time.

Types of data collections in chemistry

Dictionaries This includes both classical lists of definitions of terms, and "chemical dictionaries" which have alphabetical lists of compounds, with various kinds of data.

Encyclopedias Encyclopedias have substantial articles on relevant topics, usually in alphabetical order, usually with a significant bibliography of the source literature.

Physical data collections (including spectra collections) Physical data collections can take many different forms, depending on the objective of the editor. Some are ordered by compound name or formula, others by the value of the property in question.

Reaction and synthesis guides These may collect preparations of individual compounds, applications of individual reagents, or general methods, grouped by type of reaction, type of starting material or type of product.

Analytical methods guides These may deal with specific or general techniques, grouped by analyte, matrix, or method.

Health, safety, toxicity guides

Comprehensive works These are usually ongoing series, attempting to summarize all of a given area of chemistry. Good examples include the *Beilstein Handbook of Organic Chemistry* and the *Gmelin Handbook of Inorganic and Organometallic Chemistry*.

CRC Handbook of Chemistry and Physics (Ref Desk QD 65 .H3)

Familiar source; published annually but usually changes little from one year to the next.

Variety of useful physical and chemical data, with some references. Tables are grouped in broad subject sections. Arrangement within tables varies.

Most frequently used for tables of organic compounds and inorganic compounds, which contain data on melting points, boiling points, density and solubility among others.

Note that both tables have synonym indexes following the table.

Not very systematic in choice of data, and indexing can be inconsistent.

CRC is now publishing a Web version of the Handbook as part of [ChemNetBase](http://www.hbcnetbase.com/) at <http://www.hbcnetbase.com/>.

The electronic version may be browsed by table of contents, or searched by text term. It may also be searched by physical property values (requires a browser capable of handling Java 2 applets) and allows you to sort tabular information in a variety of ways. To use, select "Substance/Property Search", then pick the property or properties you wish to search by, then pick the appropriate operator (=, >, <, etc.), then enter the values you wish to search.

The electronic version may be searched freely by anyone, but display of data requires a subscription. The UC system has a current subscription to this version.

Merck Index (RS 356 .M4)

Published by Merck Pharmaceuticals, with data primarily on organics, strongest on drugs (surprise!).

Includes physical data, preparation references., toxicity and uses.

Arranged alphabetically by chemical name; well-indexed; updated irregularly.

It also contains a small number of other tables, and a section describing over 400 "name reactions" in chemistry, with reaction schemes and references.

The Merck Index is now available in a [Web version](http://www.rsc.org/Merck-Index/) from the Royal Society of Chemistry at <http://www.rsc.org/Merck-Index/>. The UC system now has a site licence for the Web version. Compound information may be searched by chemical name, CAS Registry Number, selected property values and chemical structure. Name reactions may be browsed alphabetically or searched by keyword.

Aldrich Catalog (TP 202 .A48)

More than just a catalog...

Includes basic physical data, cross-references to *Beilstein*, *Merck* and *Fieser*, and safety information.

Arranged alphabetically, with indexes by molecular formula and CAS Registry Number.

The [combined Aldrich and Sigma chemical catalogs](#) are searchable on the Web at <http://www.sigmaaldrich.com/> The online version additionally includes links to Aldrich's FT-IR, Raman and proton NMR spectra, as well as Materials Safety Data Sheets for each compound. If your browser can handle Java applets, you can also search by structure or substructure (with or without stereochemistry.)

Note that in both print and online versions, a single compound may appear in a number of different product records, usually representing various grades of purity. Note also, physical property data is usually only listed for the highest grade version of a given compound.

See also other chemical companies catalogs, both in print and on the Web. Check [Chemistry & Biochemistry: Chemical Suppliers](#) at <http://guides.library.ucsb.edu/content.php?pid=50952&sid=452146>.

[ChemBioFinder.com](#)

<http://chembiofinder.cambridgesoft.com/>

This database, provided by PerkinElmer Informatics (formerly CambridgeSoft), provides basic physical data and structure diagrams.

It also has links to websites containing other data for a some chemical compounds.

It is searchable by name, molecular weight, molecular formula, CAS Registry Number.

With a free browser plug-in, you can also search by structure.

The basic ChemBioFinder site is freely available to all users, but is advertiser-supported. Also, you must register (free) on the site.

Perkin-Elmer also offers an ad-free subscription version under the name ChemINDEX.

Encyclopedia of Chemical Technology (TP 9 .E685 1991)

Commonly referred to as "Kirk-Othmer" after its early editors.

Wide-ranging, authoritative encyclopedia of chemical and process information

4th edition is now complete in 25 volumes plus supplement and index; 3rd and earlier editions still useful. Wiley is now releasing a 5th edition, but we have no plans to purchase it in print.

Very strong on industrially important chemicals.

Good subject indexing, cross-references and bibliographies.

Wiley has made this encyclopedia available in a browsable and searchable [Web version](#) at <http://onlinelibrary.wiley.com/book/10.1002/0471238961>. The UC system has a subscription. Note that articles are updated online as new versions are completed. Eventually, the online version will reflect the completed print 5th edition.

Other important encyclopedias of chemical engineering are: *Encyclopedia of Chemical Processing and Design*, aka "McKetta's", SEL Ref TP 9 .E66 *Ullman's Encyclopedia of Industrial Chemistry*, SEL Ref TP 9 .U57 1985 Ullman's is also available in a [Web version](#) at <http://onlinelibrary.wiley.com/book/10.1002/14356007>, and UC has a subscription to it as well.

Polymer Science: A Comprehensive Reference (http://www.sciencedirect.com/science/referenceworks/9780080878621)

Very recent ten-volume reference work on a wide range of current topics in polymer science, including volumes on nanostructured polymers and polymers for sustainability and green energy.

UCSB has this only in [online form](#).

Encyclopedia of Polymer Science and Engineering (SEL Ref TP 1087 .E46 2003)

Sister publication to *Encyclopedia of Chemical Technology* above.

Covers polymer science in great detail, with thorough indexing, good cross-references and excellent bibliographies.

This new 12 volume 3rd edition is organized interestingly: rather than alphabetically listing articles from Volume 1 to Volume 12, the volumes are grouped in three sets of four. For best results, consult the index in Volume 12 to find relevant articles.

UCSB has access [Web version of the 4th edition](#) of this encyclopedia at <http://onlinelibrary.wiley.com/book/10.1002/0471440264>.

Polymeric Materials Encyclopedia (SEL Ref TP 1110 .P65 1996)

Relatively recent, 12 volume work on polymeric materials; covers both natural and synthetic polymers, both specific compounds and classes of compounds; preparations, reactions and properties; processes and applications.

Well referenced and indexed.

Encyclopedia of Materials: Science and Technology (SEL TA402 .E53 2001)

This is a recent source for the increasingly broad and multidisciplinary field of materials.

The [Elsevier electronic version](#) (<http://www.sciencedirect.com/science/referenceworks/0080431526>) of what is a 10,000 page, 11 volume print work, may be searched by article author, theme, subject or cited author. UCSB has access to the electronic [Encyclopedia of Materials: Science and Technology](#), however, via [Knovel](#) at <http://app.knovel.com/web/toc.v/cid:kpEMSTV001/viewerType:toc/?>

"Landolt-Bornstein" (QC 61 .L3 1961)

Actual title: *Numerical Data and Functional Relationships in Science and Technology*

Largest single collection of purely physical data -- over 300 volumes and sub-volumes in New Series alone.

The series went through six editions which superseded one another. The "New Series" doesn't replace the 6th edition. Both are listed in

the indexes.

New Series is in both German and English; 6th Ed. is entirely in German.

The New Series is subdivided by broad subject categories into "series":

Series 1: Elementary particles, nuclei and atoms

Series 2: Molecules and free radicals

Series 3: Condensed matter (i.e., crystal and solid state physics)

Series 4: Physical chemistry

Series 5: Geophysics

Series 6: Astronomy and Astrophysics

Series 7: Biophysics

Series 8: Advanced materials and technologies

Lots of data, but poorly indexed in the print version. There are overall subject indexes, but they're not very good.

If you have a particular substance in mind, consult the three-volume substance index, then scan list for available property data.

UCSB's print volumes and indexes are currently in storage at the Library Annex, and may be requested from there.

Springer had produced a Web edition through MetaPress.com. It was now truly text-searchable, though not searchable by numeric ranges, and it does display the full text of all the (300+) volumes of the New Series. Most recently, Springer has revamped the electronic version, and markets it as [SpringerMaterials](http://www.springermaterials.com/) (<http://www.springermaterials.com/>) UCSB does not currently have access to this version.

The University of California has access to an [archival collection of Landolt-Börnstein volumes](http://uclibs.org/PID/8782), comprising the volumes published from 1918-2009 at <http://uclibs.org/PID/8782>. At present, the volumes are listed by the titles of individual volumes. Eventually, they will be grouped into the subject series listed above for easier browsing. Each volume is divided into section-by-section PDF files. There is no full-text or data searching available in the Portico archive

[Encyclopedia of Chemical Physics and Physical Chemistry](#)

This encyclopedia, published by the Institute of Physics (the primary society for physicists in the UK) in 2001, comprises three volumes on fundamentals, methods and applications in chemical physics and physical chemistry. UCSB has this work only in electronic form, via [Knovel](#).

***International Critical Tables of Numerical Data, Physics, Chemistry and Technology* (SEL Q 199 .N27)**

This collection of property tables, published in 1926, is still highly regarded as a source of useful property data over 80 years later. Recently, an [electronic version](http://app.knovel.com/web/toc.v/cid:kpICTNDPC4/viewerType:toc/?) <http://app.knovel.com/web/toc.v/cid:kpICTNDPC4/viewerType:toc/?> was made available free of charge to academic institutions by [Knovel, Inc.](#) The electronic version can be searched by keyword, or by links from the original subject index. Some of the tables have been "knovelized" to make them available as sortable, filterable spreadsheet-like tables.

Other "free" Knovel data collections include: [Knovel Critical Tables](#), and [Smithsonian Physical Tables](#). All Knovel digitized reference works may be searched for no charge, but display of the data in most requires a paid institutional subscription.

"Comprehensive Chemistry" Series

(various call numbers, see below)

Pergamon Press (a division of Reed Elsevier) publishes a number of sets in various subject areas containing review articles by eminent researchers.

Within each set, the article chapters are grouped into volumes by broad subject area.

The indexing is mediocre and you may have to check several possible headings to find the desired information.

Elsevier has begun to make some of these titles available in electronic form on its [ScienceDirect](#) platform (see <http://www.sciencedirect.com/>. Click on Books, then on Reference Works, for a complete list.)

Some of the titles have also been made available via [Knovel](#) or Gale. See below for titles to which UCSB has access.

Currently available titles in chemistry and related fields are:

[Comprehensive Biomaterials](#) (online only at UCSB)

[Comprehensive Biophysics](#) (online only at UCSB)

[Comprehensive Biotechnology, 2nd ed.](#) (online only at UCSB; 1st edition in print at **SEL Ref TP 248.2 .C66 1985**)

[Comprehensive Chemometrics](#) **SEL Ref QD 75.4 .C45 C65 2009**

[Comprehensive Chirality](#) (online only at UCSB)

[Comprehensive Composite Materials](#) **SEL TA 418.9.C6 C6344 2000**

[Comprehensive Coordination Chemistry](#) **SEL Ref QD 474 .C65 1987**

[Comprehensive Coordination Chemistry II](#) **SEL Ref QD 474 .C65 2004**

[Comprehensive Glycoscience](#) **SEL Ref QP 601 .C65 2007**

[Comprehensive Heterocyclic Chemistry](#) **SEL Ref QD 400 .C65 1984**

[Comprehensive Heterocyclic Chemistry II](#) **SEL Ref QD 400 .C65 1996**

[Comprehensive Inorganic Chemistry](#) **SEL Ref QD 151.2 .C64**

[Comprehensive Inorganic Chemistry II](#) (online only at UCSB)

[Comprehensive Medicinal Chemistry](#) **SEL Ref RS 402 .C65 1990**

[Comprehensive Medicinal Chemistry II](#) **SEL Ref RS 402 .C65 2007**

[Comprehensive Membrane Science and Engineering](#) (online only at UCSB)

[Comprehensive Nanoscience and Technology](#) (online only at UCSB)

[Comprehensive Natural Products Chemistry](#) SEL Ref QD 415 .C63 1999
[Comprehensive Natural Products II](#) (online only at UCSB)
[Comprehensive Organic Chemistry](#) SEL Ref QD 245 .C65
[Comprehensive Organic Functional Group Transformations](#) SEL Ref QD 262 .C534 1995
[Comprehensive Organic Functional Group Transformations II](#) SEL Ref QD 262 .C534 2005
[Comprehensive Organic Synthesis](#) SEL QD 262 .C535 1991
[Comprehensive Organometallic Chemistry](#) SEL Ref QD 411 .C65 1982
[Comprehensive Organometallic Chemistry II](#) SEL Ref QD 411 .C652 1995
[Comprehensive Organometallic Chemistry III](#) SEL Ref QD 411 .C653 2007
[Comprehensive Polymer Science](#) SEL Ref QD 381 .C66 1989
[Comprehensive Renewable Energy](#) (online only at UCSB)
[Comprehensive Semiconductor Science and Technology](#) (online only at UCSB)
[Comprehensive Supramolecular Chemistry](#) SEL Ref QD 411 .C66 1996
[Comprehensive Toxicology](#) SEL Ref RA 1199 .C648 1997

***Encyclopedia of Inorganic Chemistry* (SEL Ref QD148 .E53 1994)**

Fairly recent; mixture of short "definition" articles with longer review articles by noted authors with good bibliographies.

Covers inorganic, bioinorganic, organo-metallic and coordination chemistry

Alphabetical organization, with thematic list in the foreword, subject index and list of contributors.

UCSB has online access to the new version, [Encyclopedia of Inorganic and Bioinorganic Chemistry](#) at <http://onlinelibrary.wiley.com/book/10.1002/9781119951438>

***CRC Handbook of Data on Organic Compounds (HODOC)* (SEL QD 257.7 .H36)**

Multi-volume set gives structures, basic physical properties of organic (and some organometallic) compounds.

Includes references to *Beilstein* and to Sadtler spectra collections.

Alphabetical order. Indexes for synonyms, formulas, spectral peaks, CAS Registry #'s. Now in 3rd edition.

An electronic version, [Properties of Organic Compounds](#) is available at <http://www.chemnetbase.com/scripts/pocweb.exe>, part of CHEMnetBASE. It is searchable by name or chemical property, and with the proper structure-drawing plugin, by substructure. The electronic version gives spectral peaks, but not always the Sadtler cross-references.

***Handbook of Physical Properties of Organic Compounds* (SEL Ref QD 257.7 .H374 1997)**

Single volume, gives structure and data important to environmental fate of compounds (mp, bp, water solubility, octanol-water partition coefficient, vapor pressure, pKa, Henry's Law constant, and atmospheric hydroxyl radical reaction rate constant), and references.

Arranged by CAS Registry Number, with name and molecular formula indexes.

"Dictionary of Compounds" Series

CRC Press publishes a variety of "dictionaries" of compounds (formerly published by Chapman-Hall.)

They give structure diagrams, basic physical data (on both the compound and significant derivatives), and references for other information.

Alphabetical arrangement; well-indexed, including CAS Registry #'s.

Current sets include:

Dictionary of Organic Compounds, 6th ed. SEL QD 251 .D5 1996

Dictionary of Natural Products SEL QD 415 .A25 D53 1994

Dictionary of Inorganic Compounds SEL QD 148 .D53 1992 Note: Unlike the other titles, this one is arranged by molecular formula, with the elements arranged alphabetically.

Dictionary of Organometallic Compounds, 2nd ed. SEL QD 411 .D53 1995

Dictionary of Organophosphorus Compounds SEL SEL QD 412 .P1 E36 1988

Dictionary of Antibiotics SEL RS 431 .A6 D53 1988

Dictionary of Drugs SEL RS 51 .D479 1990

Dictionary of Analytical Reagents SEL QD 77 .D498 1993

CRC has a Web version of the [combined chemical dictionaries](#) as part of ChemNetBase at <http://www.chemnetbase.com/scripts/ccdweb.exe>. The UC system has a subscription to this resource. Like "Properties of Organic Compounds" mentioned above, it is searchable by name, chemical property or (with plug-in) by substructure.

"Houben-Weyl" *Methoden der Organischen Chemie* (QD 258 .M4)

A very comprehensive series on organic methods, with periodic supplements.

Organized by chemical classes.

Entirely in German, until relatively recently.

Now publishing specialized sets, e.g. on stereoselective reactions. *Stereoselective Synthesis* SEL QD 258 .M4 1952 v.E21 parts 1-10 Published in 1996, this is an excellent compendium of methods for synthesizing and characterizing stereospecific compounds, with good indexing.

Starting in 2002, "Houben-Weyl" was relaunched under the title [Science of Synthesis](#). This is an electronic version of a handbook of organic synthetic methods, in two parts: **Science of Synthesis** contains 48 volumes, covering the fields of Organometallics; Heteroarenes and Related Ring Systems; Compounds with Four Carbon-Heteroatom Bonds e.g. Carbonic Acids, Imidic Acids etc.; Compounds with Three Carbon-Heteroatom Bonds e.g. Nitriles, Isocyanides, and Derivatives, Amides and Derivatives, Peptides, Lactams, Thio-, Seleno- and Tellurocarboxylic Acids and Derivatives, Compounds with Two Carbon-Heteroatom Bonds e.g. Ketones, and Heteroatom Analogues of

Aldehydes and Ketones, Compounds with One Saturated Carbon-Heteroatom Bond (e.g. halogens) and Compounds with All-Carbon Functions. It is browsable by the table of contents, and may be searched by chemical name or chemical structure. The **Houben-Weyl Archive** (1909 to 2004) provides immediate access to 146 000 product specific experimental procedures, 580 000 structures, and 700 000 references in all fields of synthetic organic chemistry - dating back to the early 1800s. It may be browsed by table of contents, or searched for name reactions. Most of the earlier volumes are in German. UCSB has a subscription to this resource.

Organic Reactions (SEL QD 251 .O68)

Annual publication with review articles on important synthetic methods.

Articles are published in no particular order, but the series is well-indexed, with cumulative author and chapter/topic indexes in each volume for all the preceding volumes.

UCSB has access to an [electronic version](#) on the Web (see: <http://onlinelibrary.wiley.com/book/10.1002/0471264180>). It currently all volumes of the printed work. The articles are not listed by volume, but may be browsed by article title or reaction type, and searched by keyword or structure.

Organic Syntheses (QD 262 .O68)

Annual publication with **tested** syntheses of organic and organometallic compounds.

Gives detailed descriptions of synthetic techniques, reagents, yields and safety aspects.

Well-indexed (authors, compound names, reaction types, molecular formulas)

Collective volumes include revised and updated syntheses from annual volumes. There is a cumulative index for the first eight collective volumes.

The publishers, in collaboration with Wiley and CambridgeSoft, has released a **FREE Web version** at <http://www.orgsyn.org/> With a free chemical drawing plug-in available at the Web site, the online version is substructure searchable.

Wiley has also released a somewhat more up-to-date [subscription version](#). Note that articles in this Wiley reference work (and many others) are available on a pay-per-view basis to individual users.

Inorganic Syntheses (SEL Ref QD 151 .I5)

A less-than-annual publication, similar in format to *Organic Syntheses*

Covers inorganic and organometallic compounds (including boranes, synthetic metals, superconductors)

No collective volumes, but the indexes cumulate every five volumes. Wiley has created an online version of [Inorganic Syntheses](#) at <http://onlinelibrary.wiley.com/bookseries/10.1002/SERIES2146>. Chapters are available as PDF files, and may be searched by chapter title but they are not searchable as a true database like *Organic Syntheses* (yet). UCSB does not have an online subscription.

Fieser and Fieser's Reagents for Organic Synthesis (SEL Ref QD 262 .F5)

Classic series reporting on new reagents and new uses for old reagents.

Published less-than-annually.

Alphabetical list of reagents, with author and subject index.

Cumulative index for Vols. 1-12.

Wiley is creating an [electronic version](#) of this series at <http://onlinelibrary.wiley.com/book/10.1002/9780471264194>. Articles may be browsed by title, or searched by full text keyword. UCSB does not have a subscription to this as yet. It is rumored that Wiley may incorporate "Fieser" in with other synthesis-related series which they publish, but no such product has been released yet.

Encyclopedia of Reagents for Organic Synthesis (SEL Ref QD 77 .E53 1995)

Recent multi-volume set, listing compounds in alphabetical order

Gives physical data and brief, but detailed description of uses

Excellent references and indexing (compound name, formula, type of reaction)

Wiley has released a browsable and searchable electronic version called [e-EROS](#); see <http://onlinelibrary.wiley.com/book/10.1002/047084289X>. The electronic version of EROS is structure, substructure and reaction-searchable via a Java applet. The online version is the current edition, and is updated periodically, though some articles still date to the first edition.

Spectra Collections

UCSB Library has a variety of collections of spectra, some one volume, some multivolume, including IR, NMR, UV, powder diffraction, etc.. Most are located at either QC 435-765 or QD 95-96.

Some have general coverage, some deal with specific classes of compounds.

In ascending order of size and complexity, the main SEL Ref Area spectra collections are:

Multi-type Spectra Collections

Integrated Spectral Data Base System (SDBS)

http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng This site, from the National Institute of Materials and Chemical Research in Japan, contains full spectra and, in many cases, peak assignments for about 33,000 compounds, including about 24,000 electron-impact mass spectra, 13,000 ¹³C NMR, 14,700 proton NMR, 51,100 Fourier transform (FT) IR, 3,500 Raman and 2,500 ESR spectra. Peak assignments are provided, where possible, for the NMR spectra. The database is searchable by compound name, CAS

Registry Number, molecular formula and NMR or IR peaks. The database is free to the public, but users are asked to download no more than 50 spectra per day without specific permission of the site owners.

NIST Chemistry Webbook

<http://webbook.nist.gov/> Among other data, NIST Chemistry Webbook has IR spectra for over 16,000 compounds, mass spectra for over 15,000 compounds, UV/visible spectra for over 1,600 compounds and electronic and vibrational spectra for over 5000 compounds which may be searched in a variety of ways, displayed and printed. Note that the variety of data available here is growing; well-worth checking for a wide variety of data. The Webbook may also be searched by keyword, property or chemical name along with a large number of NIST databases at the [NIST Data Gateway](http://srdata.nist.gov/gateway/). <http://srdata.nist.gov/gateway/>.

Infrared

***Aldrich Library of Infrared Spectra*, 2nd ed. (SEL Ref QD 96 .I5 P67 1981) *Sadtler Handbook of Infrared Spectra* (SEL Ref QC 453 .S73 1978)**

NMR

***Sadtler Handbook of Proton NMR Spectra* (SEL Ref QC 490 .S23) *Sadtler Guide to Carbon 13 NMR Spectra* (SEL Ref QC 762 .S28 1983) *Aldrich Library of NMR Spectra* (3 volumes, Ref QC 762 .P69) *Aldrich Library of ¹³C and ¹H FT NMR Spectra* (3 volumes, Ref QD 96 .F68 P67 1993) *Handbook of Proton-NMR Spectra and Data* (10 volumes + index, Ref QC 762 .H33 1985)**

***Encyclopedia of Nuclear Magnetic Resonance* (QC 762 .E53 1996)**

Not a spectra collection; gives articles on techniques, applications, types of substances on which NMR has been done.

Vol. 1 is all on "historical perspectives" on NMR.

Excellent references and indexing.

UCSB has online access to a newer edition, the [Encyclopedia of Magnetic Resonance](http://onlinelibrary.wiley.com/book/10.1002/9780470034590) at <http://onlinelibrary.wiley.com/book/10.1002/9780470034590>

***Encyclopedia of Spectroscopy and Spectrometry* (SEL Ref QD 95 .E55 2000)**

New three volume work, covers all forms of spectroscopy.

Articles on particular types of spectroscopy, and on types of substances which one might examine.

Well indexed; lots of "further reading" with each article.

Volume 3 contains lots of useful tables in the appendices.

***Encyclopedia of Computational Chemistry* (QD 39.3 .E46 E53 1998) <http://onlinelibrary.wiley.com/book/10.1002/0470845015>**

Relatively recent five volume work, covering all areas of computers in chemistry: structure-activity relationships, molecular modeling, electronic structure modeling...you name it.

Good indexing; lots of references.

UCSB has access to the online version of this encyclopedia.

***Encyclopedia of Catalysis* (QD 505 .E53 2003) <http://onlinelibrary.wiley.com/book/10.1002/0471227617>**

Fairly recent six-volume work with alphabetically-arranged articles on the most significant aspects of homogeneous, heterogeneous, asymmetric, biomimetic, and biological catalysis.

UCSB has access to the online version of this encyclopedia.

***Encyclopedia of Analytical Chemistry* (SEL Ref QD 71.5 .E52 2000)**

Relatively recent and comprehensive.

The 15 volume set devotes its first ten volumes to areas of chemical analysis (e.g., Chemical Weapons Chemical Analysis; Environment: Water and Waste; Peptides and Proteins; Surfaces) and the last five volumes to methods (e.g., Atomic Spectroscopy; Liquid Chromatography; Radiochemical Methods).

The articles are detailed, by experts in their fields, with good references and cross-referencing.

***Encyclopedia of Analytical Science, 2nd ed.* (SEL Ref QD 71.5 .E53 2005)**

Excellent relatively recent reference for analytical chemistry. Its articles cover:

Techniques, like "atomic absorption spectroscopy"

Analytes, like "antimony", "asbestos", "carbohydrates"

Matrices, like "blood", "ceramics"

Classes of analysis, like "bioprocess analysis", "forensic science"

Well-indexed and cross-referenced.

***Comprehensive Analytical Chemistry* (QD 75. W5)**

A 43 volume (and growing) series, each devoted to a particular analytical technique. (UCSB currently has 1-37.)

Older volumes may be in storage during construction; if so, use interlibrary loan.

Excellent source of detailed information on the techniques covered. Since the series started in 1959, some of the earlier volumes are rather dated.

Current Protocols (Various call numbers)

The Current Protocols series are laboratory manuals considered a benchmark for scientific research methods. With their regular updates, these publications constantly evolve and change to meet the needs of the scientific research community. They include:

Step-by-step protocols with annotations that alert you to special considerations, tips, and optional procedures.

Alternate and support protocols to accommodate different equipment and desired results.

Materials lists for each protocol to ensure you have everything you need before you start work.

Detailed recipes for reagents, solutions, and culture media.

Expert commentaries filled with scientific insight, including general background, troubleshooting instructions, and planning considerations.

Tables and figures to clarify complex procedures.

Appendices filled with useful reference material.

The University of California has a subscription to most of the Protocols series in online form, including:

[Current Protocols in Bioinformatics](#)

[Current Protocols in Cell Biology](#)

[Current Protocols in Cytometry](#)

[Current Protocols in Human Genetics](#)

[Current Protocols in Immunology](#)

[Current Protocols in Molecular Biology](#)

[Current Protocols in Neuroscience](#)

[Current Protocols in Nucleic Acid Chemistry](#)

[Current Protocols in Pharmacology](#)

[Current Protocols in Protein Science](#)

[Current Protocols in Toxicology](#)

The protocols are browsable by Table of contents or keyword searchable with stemming (truncation) and a subject thesaurus.

[Hazardous Substances Data Bank \(HSDB\)](#)

<http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>

This database, from the National Library of Medicine, indexes over 5000 compounds. It is searchable by chemical name, CAS Registry Number, or keyword.

Categories of data include: Human Health Effects, Emergency Medical Treatment, Animal Toxicity Studies, Metabolism/Pharmacokinetics, Pharmacology, Environmental Fate/Exposure, Chemical/Physical Properties, Chemical Safety & Handling, Occupational Exposure Standards, Manufacturing/Use Information, Laboratory Methods, Special References, and Synonyms and Identifiers. References are provided for all data, as well as information on when the record was updated.

Note that the quantity of information varies considerable with how much the compound has been studied for health and safety.

Sax's Dangerous Properties of Industrial Materials (T 55.3 .H3 L494 2005)

Excellent collection of info, especially LD50 and related data

Some information, especially references, are heavily abbreviated. Consult the guide in Vol. 1 to interpret the notations.

Alphabetical by substance. Good synonym index, CAS Registry Number index.

Hazardous Substances Resource Guide (SEL Ref T 55.3 .H3 H444 1997)

Good source with effects on humans

Lists of useful publications, organizations

Hazards in the Chemical Laboratory, 4th ed. (SEL Ref QD 51 .H35 1986)

Classic book on lab safety, with a British bent.

CRC Handbook of Laboratory Safety, 3rd ed. (SEL Ref QD 51 .H27 1990)

Everything you always wanted to know about setting up and operating a laboratory safely.

Other Data Collections on the Web

Many classic data collections are not available on the Web because their publishers are making good money off the print versions, and they haven't figured out how to best make money off of Web versions.

However, there are some good collections on the Web, mostly from government sources, academic sources, or commercial firms seeking to demonstrate the usefulness of their products.

In addition to sites mentioned above, see also [UCSB Library's Chemistry & Biochemistry Help by Subject](#) page at <http://guides.library.ucsb.edu/chemistry> for some examples.

For references in specific subdisciplines, see also the following specialized guides: [Analytical Chemistry](#) [Biochemistry](#) [General Chemistry](#) [Inorganic Chemistry](#) [Organic Chemistry](#) [Physical Chemistry](#) [Chemical Engineering](#)

