

CHEMISTRY INFORMATION RESOURCES AT CALTECH

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TRANSLITERATION

The transliteration of Cyrillic names, to the Latin alphabet, is complicated by the use of three different schemes (in the U.S. alone) and further problems arise in German and French indexes (1a). Zhanov, for example, in an English language index may be written as Shdanow in a German language index and Jdanoff in a French language index. A comparative table of transliteration schemes is available (1b). There are also Japanese transliteration variations (e.g. Oe or Ohe) that depend on personal preference. Searching SciFinder for Liubinskii (with the alternative spelling turned on) retrieves Lyubinskii.

CLAS	PubMed	CA(print)	WoS	SFS
Izvestiia	Izvestiia	Izvestiya	Izvestiya	Izvestiya
Liubinskii	Liubinskii	Lyubinskii	Lyubinsky	L(i/y)ubinskii

UMLAUTS, etc. or HYPHENATED OR COMPOUND NAMES

Computer programs generally can not accommodate umlauts and the handling of apostrophes and compound or hyphenated names is often inconsistent. For example:

Published as	Schroder	Ostvold	O'Brian	Brown-Wensley	Van der Waals
CLAS	Schroder	Ostvold	O'Brian	Brown-Wensley	Waals, van der
Medline	Schroder	Ostvold	O'Brian	Brown-Wensley	van der Waals
Web of Science	Schroder	Ostvold	OBrian	Brownwensley	Vanderwaals
WoS(1998+)	Schroder	Ostvold	O'Brian	Brown-Wensley	Van der Waals
SFS (1907-61)	Schroder	Ostvold	O'Brian	Brown-Wensley	Van der Waals
SFS (1962-96)	Schroeder	Oestvold	O'Brian	Brown-Wensley	Van der Waals
SFS (1997+)	Schroder	Ostvold	O'Brian	Brown-Wensley	Van der Waals

CA has changed the way it handles umlauts over the years. In the CA print Author Index from 1907-61, names were printed with umlauts but filed as if spelled out. From 1961-1996, names with umlauts were generally spelled out. Beginning in 1997, umlauts are ignored as they are in the (pre-1961) SciFinder Scholar records.

Searching SciFinder (with the alternative spelling turned on) for – H. A. Schroder retrieves 60 names including – H.A. Schroeder. Searching for – K. A. Brown-Wensley retrieves 82 names and highlights Brown Wensley. The list also lists all the K. and K.A. Brown's which is helpful, since Ms Brown-Wensley changed her name back to Brown.

Although apostrophe, compound and hyphenated names appear in CA print Author Index as shown above, they are filed as if they were condensed (e.g. OBrian).

EDITING OF AUTHOR NAMES: CHANGES IN PRACTICE

Currently, an author name will appear in the Chemical Abstracts database and services exactly and as fully as it is presented in the original document. A misspelling will be corrected if it is recognized. Most diacritical marks appearing in the original documents are eliminated (i.e., they are not transliterated). Author names that do not appear in the Roman alphabet in the original source documents are transliterated according to the particular methods described in the Introduction to the CA Author Index. Variations in names may occur in the database owing to differences in the original publications (e.g., initials for the first and/or middle names versus full first and/or middle names, or the use of different transliteration schemes). Users of CAS services are encouraged to **consider alternative forms of author names** when searching in the printed or electronic services.

Historically, the first issues of Chemical Abstracts presented author names exactly as they appeared in the original documents complete with diacritical marks. The practice of transliterating letters with diacritical marks and special characters with English equivalents was introduced in 1961 and continued thru 1996. Thus, for example, the Germanic letter "u" with an umlaut was replaced by "ue". Consistency of practice application has varied. Please note that publisher practices with diacritical marks also vary and, consequently, varying forms of the names will appear in the databases. Please also note that umlauts are NOT transliterated in the pre-1961 online records.

Chinese Names: A change in transliteration of author names occurred in 1982 when CAS began to use the Pinyin system for transliterating author names appearing in publications originating in the People's Republic of China, while retaining the Wade-Giles system for Chinese-language documents from Taiwan and other countries. This change was made because the Pinyin scheme had been adopted by the PRC as its official method of transliteration. The use of these two Chinese transliteration schemes continues today.

CASSI (Chemical Abstracts Service Source Index) is a listing of publications abstracted by CAS from 1907+ alphabetically arranged by their ISO abbreviations. It is particularly useful for identifying English translations of Russian language journals. It also provides see-references from translated titles, such as: Progress in Biochemistry and Biophysics (used in WoS) to their transliterated titles Shengwu Huaxue (used in CLAS & SciFinder Scholar). Entries in CASSI are filed alphabetically, letter-by-letter, by ISO journal abbreviations (which are printed in **bold face**).

Zeitschrift fuer **Chemie**
Zeiss Information
Zhurnal **Obshchei Khimii**
Zoon
Zeitschrift fuer **Physik**

The CAS DDS Title Search database <http://www.cas.org/Support/DDS/ddssearch.html> contains serials currently received at Chemical Abstracts Service and nonserials whose publication date is within the past ten years. DDS Title Search provides only the full title of a publication but is searchable by keywords (and keyword strings within words), CODEN, ISSN, or ISBN.

BEILSTEIN (1910) & (Crossfire) JOURNAL ABBREVIATIONS

(1910)	(Crossfire)	Correct title
A.	justus liebig's ann.chem.	
A. ch.	ann.chim.(Paris)	Ann. Chim. Phys.
Am. Soc.	j.am.chem.soc.	
Ann. d. Physik	ann.phys.(Leipzig)	
Ar.	arch.pharm.	
B.	chem.ber.	Ber. Dtsch. Chem. Ges.
Bl.	bull.soc.chim.fr.	
C.	chem.zentralbl.	
C. r.	c.r.hebd.seances acad.sci.	
Fr.	fresenius z.anal.chem.	
G.	gaz.chim.ital.	
J.	jahresber.fortschr.chem. ...	
J. pr.	j.prakt.chem.	
M.	monatsh.chemie	
R.	recl.trav.chim.pays-bas	
R. A. L.	atti accad.naz.lincci cl.sci.phys.mat.nat.rend	
Soc.	j.chem.soc.	
Z. a. Ch.	z.anorg.allg.chem.	Z. Anorg. Chem.

NAMING & INDEXING OF CHEMICAL COMPOUNDS (SFS)

The Chemical Abstracts Index Names in SFS (CA Index Guide, Appendix 4) follow a very non-obvious rule. Substituent names (e.g. ethyl, iodo, methyl, chloro, methoxy, methyl) are placed in alphabetical order, and only then are both the multiplicative prefixes (di, tri, etc.) and alpha/numeric locants (e.g. 1, 4, N, etc.) placed in front of each substituent name. For example:

N-ethyl-4-iodobenzenamine
4-iodo-N-methylbenzenamine
1,2,3,4-tetrachloro-5-methoxy-6,7-dimethylnaphthalene

These 'direct' names (which are found in the Merck Index), however, are generally not searchable. For indexing purposes, Chemical Abstracts inverts the index name and alphabetically arranges them (ignoring alpha/numeric locants) in the CA (print) Chemical Substance Index. The SFS Registry File generally only lists compound names in their inverted form.

Benzenamine, N-ethyl-4-iodo-
Benzenamine, 4-iodo-N-methyl-
Naphthalene, 1,2,3,4-tetrachloro-5-methoxy-6,7-dimethyl-

IUPAC nomenclature, while widely used, does not provide unique names. Compounds with multiple functional groups can be named in a variety of ways depending on the author's emphasis.

For example, compare: (4-iodo-phenyl)-ethyl-amine and Ethyl – (4-iodo-phenyl)-amine

Beilstein's Autonom (structures → IUPAC names) program is available with the Beilstein Commander client software. ChemWeb has a free IUPAC Naming tool that will generate IUPAC names (albeit with size & element restrictions) at: <http://www.chemweb.com/tools/acdlabs-name> (Netscape preferred).

IUPAC Nomenclature Recommendations and Glossaries for various subjects are available on their Nomenclature Page: <http://www.chem.gmw.ac.uk/iupac>

SciFinder Scholar - Synonyms

Coloring materials

caramel --- see Caramel (color)

fading of --- see Fading

removal of --- see Decolorization

Colorite 9813 Black

See Ethylene, chloro-, polymers, homopolymer [9002-86-2]
...SFS Ethene, chloro-, homopolymer

C.I. Acid Black 60

See Chromate(1-), bis [N-[7-hydroxy-8-[[2-hydroxy-5-[(methylamino)sulfonyl]phenyl]azo]-1-naphthalenyl]acetamidato(2-)]-, hydrogen [12218-95-0]

ISOMERS present additional problems. At first glance, C₂H₂Cl₂ would appear to be a fairly simple compound. However, a search of Beilstein retrieves 22 unique compounds and a search of SFS retrieves 53 unique compounds. There is a 1,1-compound, as well as a cis, a trans, & an undefined 1,2-compound, and each of these could be isotopically substituted with deuterium, tritium, C13, Cl37 or Cl38, and each of these could exist as a radical ion, carbene or polymer.

Chemical Abstracts has addressed this confusion by assigning unique identifiers (CAS Registry Numbers) to each of these different isomers. CAS RNs are analogous to ISBN numbers for books. Just as each edition or reprinting of a book requires a different ISBN, every variation in isotopic composition or stereochemical configuration will be assigned a unique CAS RN. For example:

1,1-Dichloroethene (75-35-4)

(1Z)-1,2-Dichloroethene (156-59-2)

(1E)-1,2-Dichloroethene (156-60-5)

1,2-Dichloroethene (540-59-0)

1,1-Dichloro-[2-¹⁴C]-ethene (64371-85-3)

CHEMICAL COMPOUND DATA SEARCHING

MERCK INDEX, 13th Edition, 2002

(MIL-8 QREF TABLE)

4,000 drugs and pharmaceuticals, 2,000 organic compounds/reagents, 2,000 naturally occurring substances, 1,000 elements/inorganic compounds, 1,000 agricultural compounds/biological agents.

Name, Formula, CAS RN, and Therapeutic Category & Biological Activity Indexes, Organic Name Reactions and Miscellaneous Tables (e.g. Greek alphabet, Isotonic Solutions, Latin Terms, Conversion Factors, etc.)

ALDRICH CATALOG -- PRINT

(MIL-8 QREF Table)

Over 37,000 Products. Organics, Polymer Products, Organometallics, Inorganics, etc., Compounds arranged by 'product' name. Entries include physical properties, and references to Aldrich Library of NMR or FT-IR Spectra ...

Molecular Formula, CAS RN indexes and Aldrich (Functional Group) Structure Index (e.g. Aromatic Acid Halides, Aromatic Amines, ...)

ALDRICH CATALOG -- <http://www.sigma-aldrich.com/aldrich>

Physical properties, literature and spectra references and MSDS online, with registration.

Search by Name, CAS RN, Molecular Formula, Molecular Weight & Substructure.

COMBINED CHEMICAL DICTIONARY

<http://www.chemnetbase.com/scripts/ccdweb.exe> (Netscape preferred)

The Combined Chemical Dictionary includes all the compounds contained in:

- Dictionary of Natural Products (155,000)
- Dictionary of Organic Compounds (240,000)
- Dictionary of Inorganic/Organometallic Compounds (100,000)
- Dictionary of Analytical Reagents (14,000)
- PharmaSource (38,000)

The CCD provides descriptive and numerical data on chemical, physical and biological properties, systematic and common names, literature references, structural diagrams (click on the 'benzene' ring) and connection tables (for structure searching).

Search options include: Menu Search, and Structure Search.

Searching for CAS RNs (e.g. 50-06-6) is done without hyphens (e.g. 50066), but browsing is done with hyphens. Browsing for 50066 displays a list beginning with 50256-18-3.

Browse provides a ranked list of each data set. In the MF dictionary there are sub-sets for 'all metals' and 'all-nonmetals' as well as all compounds with a given element (e.g. -ALL-Tc) and compounds with 'only CHNOX' and a variety of other element combinations.

CCD COMPOUND SELECTION:

- Basic fundamental organic and inorganic compounds ...
- Virtually every known natural product
- All currently marketed drugs
- Compounds with an established use (e.g. catalysts, solvents, reagents, etc.)
- Important coordination compounds
- Organometallic compounds representative of all important structural types
- Important biochemicals and minerals
- Miscellaneous compounds of ... active research interest

A (220 page) user manual is available, in addition to a Quick Reference Guide.
(Mil-8 REF QD5 C65 1997)

NIST CHEMISTRY WEBBOOK

<http://webbook.nist.gov/chemistry/>

Database contains ~40,000 compounds (mostly organic with a few small inorganics).

Data Type	Number of Species
Gas phase thermochemical data	6,500+
Condensed phase thermodynamic data	5,600+
Phase change thermodynamic data	13,800+
Reaction thermodynamic data	9,800+
Gas phase ion energetics data	15,600+
Gas phase ion cluster data	1,100+
IR spectrum	8,700+
Mass spectrum	12,600+
UV/Vis spectrum	400+
Vibrational & electronic energy levels	4,100+
Constants of diatomic molecules	600+
Fluid property data	33

Search Options: Formula, Name, CAS RN

Enter a chemical species name (e.g., methane)

Select the desired units for thermodynamic data: SI or calorie based

Select the desired type(s) of data:

Thermodynamic Data	Other Data
<input type="checkbox"/> Gas phase	<input type="checkbox"/> Gas phase IR spectrum
<input type="checkbox"/> Condensed phase	<input type="checkbox"/> Mass spectrum
<input type="checkbox"/> Phase change	<input type="checkbox"/> UV/Vis spectrum
<input type="checkbox"/> Reaction	<input type="checkbox"/> Vibrational and/or electronic spectrum
<input type="checkbox"/> Ion energetics	<input type="checkbox"/> Constants of Diatomic Molecules
<input type="checkbox"/> Ion cluster	<input type="checkbox"/> Henry's Law

Search Options: Ionization Energy, Electron/Proton Affinity, Vibrational/Electronic Energy Levels, Molecular Weight.

Data Set: Thermophysical Properties of selected fluids.

KIRK-OTHMER ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY

<http://www.mrw.interscience.wiley.com/kirk/>

Extensive Physical Property Data for Common Industrial compounds, e.g.

ACETIC ACID AND DERIVATIVES
ACETYLENE
ADIPIIC ACID
ALUMINUM COMPOUNDS
AMMONIA

Updated regularly, **Kirk-Othmer Online** will stay current with the latest developments in chemical technology and related fields. Articles will be updated and revised in response to actual changes and developments as they occur in the chemical industry.

Also in print (4th ed. SFL REF) (1st-3d ed. MIL-8 REF) TP9 E685

ULLMANN'S ENCYCLOPEDIA OF INDUSTRIAL CHEMISTRY

<http://www.mrw.interscience.wiley.com/ueic/>

Ullmann's describes chemical substances, ranging from raw materials and bulk products to fine and specialty chemicals, in detail.

Information on physical and chemical properties, production, applications, economic data, toxicology and occupational health is provided. Relevant patent information is supplied wherever available.

Fully international in scope and coverage and published in the English language, Ullmann's has been compiled under the supervision of a renowned global [Editorial Advisory Board](#). It contains nearly 1000 major articles, 10,000 tables, 30,000 figures, and innumerable literature sources and cross-references, written by some 3,000 authors affiliated to leading chemical companies or research institutes.

BEILSTEIN / GMELIN CROSSFIRE <http://library.caltech.edu/> (start menu) Organic / Inorganic-Organometallic compound databases for property data.

What is CrossFire?

- CrossFire is a search system with a locally loaded client interface (Beilstein Commander) which provides access to the Beilstein & Gmelin databases on the CrossFire server at the University of Wisconsin - Madison.

What is Beilstein?

- A database of 35M property records (from about 1.8M articles) for over 8M organic compounds (including salts, mixtures, peptides with <12 amino acids). Polymers or polycondensation products are not indexed.
- Covers the scientific literature from 1771 to the present.
- Reactions and properties are critically evaluated, with references to original articles.
- An electronic version of the print Beilstein Handbuch der Organischen Chemie.

What is Gmelin?

- A database of properties for over 1.4M inorganic and organometallic compounds (including coordination compounds, alloys, glasses, ceramics, and minerals).
- Covers the scientific literature from 1772 to the present.
- Properties are critically evaluated, with references to original articles.
- An electronic version of the print Gmelin Handbuch der Anorganischen Chemie.

How can I access Crossfire 2000?

- Workstations with the Commander client are available in the Millikan, SFL, Astro & Geology libraries, under the START MENU.
- Macintosh or MS Windows versions are available for downloading to Caltech workstations.

Crossfire features:

- **Substance Searching.**
Search with a name and copy the structure from the 'short display' into the structure editor. Draw the chemical structure or sub-structure or modify a copied structure and search. Beilstein has templates. Combine with property terms (e.g. NMR).
- **Reaction Searching (Beilstein only) by:**
Role (reactant and/or product) of a compound or sub-structure in a reaction.
- **Fact Searching:**
Names or portion(s) of chemical names. CAS Registry numbers. Author Names
Property values - e.g. melting point between 100 and 102 degrees, solubility, spectra ...
Dipole moment is now electrical moment. Biological function is now Pharmacological data.
- **Combination Searching** of text terms and structures or sub-structures.
- **Autonom** - a program that generates IUPAC names from an organic structures.
- **Recent additions (2000+):** Safety Data, Henry Constants, POW Constants, Easy Data Search (EDS) Options

SCIFINDER SCHOLAR 2001 <http://library.caltech.edu/> (under start menu)

Databases of articles and property data, etc. Search by substances, reactions, keywords, author names, patent numbers, company/organization names, etc. Include/exclude Medline.

SFS 2001 User Guide: <http://library.caltech.edu/publications/scifinder/scifinder2001.pdf>

CAplus <http://www.cas.org/casdb.html>

Chemical Abstracts 1907+ -- plus cover-to-cover indexing of 1,350 key chemical journals since Oct. 1994+, -- plus bibliographic information from both 'electronic' articles and from US, EP, WO patents (including machine translated abstracts for JP and DE patents), prior to CAS indexing. Records from 1907-1966 do NOT include CA Index Terms nor Registry Numbers from 1907-56.

Registry File <http://www.cas.org/casdb.html>

A chemical structure and dictionary (CA Index Name, synonyms, CAS RN or MF) database - 1957+. Currently lists nearly 19M organic and inorganic compounds and over 16M biosequences. Provides links to 'Commercial Availability' and 'Regulated Chemicals Listing'. ACD calculated property data provided for over 5M organic compounds. 'Dictionary' searching is often faster than structure searching and avoids problems of trying to limit the retrieval from a structure search, which often contains multi-component substances because of SFS' philosophy of 'maximizing retrieval'. SFS 2001 offers: Additional Options dialog box to exclude: mixtures, isotopes, polymers, etc.

ChemCats <http://www.cas.org/CASFILES/chemcats.html>

Commercially available chemical compounds and suppliers. Requires a 'compound' search, with Registry File records providing links to ChemCats/ChemList. Search 'Chemical Substance or Reaction' (it will be much faster with a CAS Registry Number) although names or molecular formulas can also be used. Clicking on the 'Commercial Sources' hotlink provides a list of suppliers, catalog date, order number, product name and description. Suppliers must be contacted directly for prices.

CA Patent Family Information <http://www.cas.org/EO/caspat.html>

Chemical Abstracts Patent Concordance/Index (1967+). Patent Family Information is only available after searching, 'getting' the references and clicking on the 'microscope icon' for a patent record, which displays the full bibliographic record including the 'Patent Family Information'.

Since CA generally abstracts European, German or WO applications first, this is a good way to find U.S. equivalents, as is the [Esp@cenet](http://ep.espacenet.com/) Worldwide database at: <http://ep.espacenet.com/>

Please note CA may provide a more descriptive patent title for U.S. patents.

CASReact <http://www.cas.org/CASFILES/casreact.html>

Reaction information (journal articles 1974+ and patents 1982+) from both the organic/organometallic sections of Chemical Abstracts and InfoChem. Only available while performing a structure search.

CHEMLIST <http://www.cas.org/CASFILES/chemlist.html>

CHEMLIST (Regulated Chemicals Listing) was originally built from data in the 1985 TSCA Inventory and supplements, and the Federal Register for 1978-1987. Sources for updates are greatly expanded (e.g. EINECS, EPA, etc.). Links from Registry File records.

The file covers 1979 to the present, with more than 227K records (4/2002). It is updated weekly.

SFS 2001 - New Features

http://www.cas.org/SCIFINDER/help/2001/SCH_Help/Ctxt_eps/default.htm

<http://www.cas.org/SCIFINDER/SCHOLAR/index.html#whatsnew>

1. Structure Searching -

a. After drawing a structure ...

Clicking 'Get Substances' and 'Additional Options' displays a dialog box that allows you to include or exclude; mixtures, polymers, isotopes, metal-containing substances and incompletely described structures. This option does not include 'multicomponent substances'.

b. After retrieving an 'Answer Set' of compounds ...

You can 'Refine' the compounds by 'Calculated Property Data' (i.e. # of hydrogen donors or acceptors, MW, Log POW, Freely Rotatable Bonds, Log DOW (i.e. Log POW as a function of pH), pKa, and solubility (in water as a function of pH)). Only about 5M compounds have the property data in their Registry File record.

2. Cited References from articles and patents are included (since 1999+). After retrieving a list of references, you can:

a. check off an article of interest and click the 'Microscope Icon' to see the cited references (many of which are 'hot linked' to their CA abstract record), or

b. check off one or more articles of interest and either:

Click 'Get Related' and then '**Cited** References'. This will display the records for all the 'hot linked' cited references in the document/s, or ...

Click 'Get Related' and then '**Citing** References' to display records (1999+) that have cited the document/s.

3. Reaction Searching has been expanded to 5M reactions -- journal articles, 1974+ and patents 1982+.

4. Registry Numbers in many document records are 'hot linked' to their Registry File records (which include CAS name, synonyms, MW, structure diagram, etc).

5. Previous enhancements (SFS 2000) included:

Company name searching/refining, functional group reaction searching, refining reactions by; yields, type, number of steps).

6. Importing Data from SciFinder Scholar to **EndNote**, ProCite and Reference Manager is described at: <http://www.cas.org/Support/scifinder2001/bibapps/download.html>

MISCELLANEOUS 'COMPOUND' RESOURCES

CHEMFINDER.COM <http://www.chemfinder.com/>

75,000 chemical compounds, from over 350 public source sites, including: biochemistry, health, medications, MSDS, pesticides/herbicides, physical properties (including manufacturer's catalogs), regulations, structures, usage, government regulatory data, and NIST. Site list is available:

<http://www.chemfinder.com/siteslist.asp>

Both a Simple Query (name, formula, molecular weight or CAS registry number) and a Structure Query (with ChemDraw or Chem3D plugins) are provided.

DIPPR <http://library.caltech.edu/databases/> (to retrieve password)

Temperature-dependent properties for over 1,600 pure chemicals

PHYSPROP (ENVIRONMENTAL) <http://esc.syrres.com/interkow/PhysProp.htm>

Environmental Physical Properties for ~25,000 Compounds. Search by Name, CAS RN.

ORGANIC SOLVENTS, 4th ed., 1986

Physical Properties .. Purification (~500 compounds). MIL-8 REF QD544.5 .R72

SOLV-DB (SOLVENTS DATABASE) <http://solvdb.ncms.org/index.html>

Properties & Cost. Search by Name, CAS RN, Sax #, MF, Category or Property Range.

MATHESON GAS DATA BOOK, 6th ed., 1980

Physical/Thermodynamic Properties for (Industrial) Gases. MIL-8 REF TP761 C65 M3

BRENDA <http://www.brenda.uni-koeln.de/>

Comprehensive Enzyme Information System. Search by Name, EC #, CAS RN, etc.

HANDBOOK OF PROTEOLYTIC ENZYMES

http://skinbark.caltech.edu/cdroms/Handbook_of_Proteolytic_Enzymes/

Grouped by catalytic type (Serine, Cysteine, Aspartic, Metallo and Unclassified)

NIST CRITICALLY SELECTED STABILITY CONSTANTS OF METAL COMPLEXES

<http://skinbark.caltech.edu/cdroms/NIST2001/>

Updated online version of Martell's Critical Stability Constants (Hydrogen considered a metal).

PHYSICAL PROPERTY DATA SEARCHING

CRC HANDBOOK OF CHEMISTRY AND PHYSICS

70th edition 1989-90, has deleted tables. Recent editions give data sources. MIL-8 QREF

INTERNATIONAL CRITICAL TABLES OF NUMERICAL DATA ..., v.1-7, 1926-30.

Comprehensive Data Compilation. MIL-8 REF Q199 N32

VNR INDEX OF CHEMICAL AND PHYSICAL DATA

Physical Property Tables, with literature references... MIL-8 QREF

LANDOLT-BORNSTEIN, 6th ed. and New Series. ~200 v., 1950-1995

Comprehensive Data Compilation. MIL-8 REF QC61 L332

<http://link.springer.de/link/service/series/0284/> (some volumes freely available)

PHYSICAL PROPERTIES OF CHEMICAL COMPOUNDS., v.1-3,1955-61 (ACS).

Thermophysical Properties (1400 organic compounds). MIL-8 REF QD473 .D7

J. PHYSICAL & CHEMICAL REFERENCE DATA - <http://ojps.aip.org/jpcrd/>

Physical Property and Spectral Data. Cumulative indexes 1-10,11-20,21-30

JPCRD SUPPLEMENTS / MONOGRAPHS (see CLAS)

e.g. Thermal Conductivity of the Elements, Atomic Transition Probabilities, etc.

THERMOPHYSICAL PROPERTIES OF MATTER, v.1-14, 1970-79

Property/Temperature Diagrams. MIL-8 REF QC171 P83

THERMOPHYS. PROPERTIES OF HIGH TEMP. SOLID MATERIALS, V.1-6, 1967

Materials with melting points above 800K or 1000F. MIL-8 REF TA418.26 P8

THERMOPHYS. PROPERTIES RESEARCH LITERATURE...GUIDE, 1900-1980. 7v.

Separate 'chapter' for each physical property. MIL-8 REF Z5853.M38 T48 1982

FINDING PHYSICAL AND CHEMICAL PROPERTIES

<http://www.library.vanderbilt.edu/science/property.htm>

THERMODEX (Property Index to Thermodynamic Handbooks)

<http://thermodex.lib.utexas.edu/>

THERMODYNAMIC DATA ... WEB SITES

http://tigger.uic.edu/~mansoori/Thermodynamic.Data.and.Property_html

SCIFINDER SCHOLAR 2001 <http://library.caltech.edu/> (under start menu)

Databases of articles. Search by property/compound class and limit to review articles.

POLYMERS AND POLYMERIC MATERIALS

POLYMER HANDBOOK, 4th edition, 1999

Tabular data on polymerization, properties, nomenclature ... MIL-8 REF QD388 P65

POLYMER DATA HANDBOOK, 1999 <http://www.oup-usa.org/pdh/>

Key data on over two hundred polymers. SFL REF TA455 P58 P485

Encyclopedia of Polymer Science & Engineering, 2nd ed., v.1-18, 1985-1990

Physical and biological properties of polymers and plastics. MIL-8 REF TP1087 E46

POLYMERIC MATERIALS ENCYCLOPEDIA, v.1-12, 1996

Synthesis, properties and applications of polymeric systems. MIL-8 REF TP1110 P65

COMPREHENSIVE POLYMER SCIENCE, v. 1-7, supp. 1-2, 1989-1996

Polymer Properties, Reactions, Processing and Specialty Polymers. MIL-8 REF QD381 C66

GE PLASTICS < www.geplastics.com/ >

Resource for engineered thermoplastic resin materials

MATWEB <http://www.matweb.com/>

Information on 26,412 materials including metals, plastics, ceramics, and composites.

Multivolume compilations:

Comprehensive Coordination Chemistry; Synthesis, reactions, properties & appl. v.1-7, 1987

Comprehensive Heterocyclic Chemistry; Structure, reactions, synthesis & uses. v.1-8, 1984

Comprehensive Heterocyclic Chemistry II. v.1-11, 1996 (literature – 1982-1995)

Comprehensive Medicinal Chemistry; Rational design, mechanistic ..., therapeutic appl. v.1-6, 1990

Comprehensive Natural Products Chemistry. v.1-9, 1999

Comprehensive Organic Chemistry; Synthesis & reactions. v.1-6, 1979

Comprehensive Organic Functional Group Transformations. v.1-7, 1995

Comprehensive Organic Synthesis; Selectivity, strategy, & efficiency ...v.1-9, 1991

Comprehensive Organometallic Chemistry; Synthesis, reactions, structures. v.1-9, 1982

Comprehensive Organometallic Chemistry II. v.1-14, 1995 (literature – 1982-1994)

Comprehensive Supramolecular Chemistry. v.1-11, 1996

Encyclopedia of Analytical Chemistry; Applications, theory and instrumentation. v.1-15, 2000

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Encyclopedia of Inorganic Chemistry. v.1-8, 1994

Encyclopedia of Nuclear Magnetic Resonance. v.1-8, 1996

Rodd's Chemistry of Organic Compounds, 1964-80. Supp.1(1975-88)Supp. 2 (1991-1999). 75 vols.

SPECTRA / SOLUBILITY / CRYSTAL STRUCTURE

SDBS <http://www.aist.go.jp/RIODB/SDBS/menu-e.html>

Integrated Spectral Data Base System for Organic Compounds (MS,NMR,IR, Raman, ESR)

SPECTRA ONLINE http://spectra.galactic.com/SpectraOnline/Default_ie.htm

Public Domain FT-IR, UV-VIS, NIR, Raman, MS, NMR, XRD, etc.

ALDRICH LIBRARY OF FT-IR SPECTRA, v.1-3, 1985

SIGMA LIBRARY ... FT-IR SPECTRA, v.1-2, 1986

ALDRICH LIBRARY..13C & 1H FT NMR SPECTRA, v.1-3, 1993

HERSHENSON'S NMR / IR / UV INDEXES (published spectra)

UV ATLAS OF ORGANIC COMPOUNDS, v.1-5, 1966-71

ABSORPTION SPECTRA ... UV & VIS (LANG), v.1-24, 1966-

SADTLER HANDBOOK ... IR / NMR / UV SPECTRA (Abridged Edition)

SADTLER .. IR (Inorganics, v.1-5 & Organometallics)

EPA/NIH MASS SPECTRAL DATABASE, v.1-4 & suppl. 1-3

SOLUBILITIES (Stephen & Stephen), 7v. 1963-1979

Binary, Ternary and Multicomponent Systems

SOLUBILITIES (LINKE/SEIDELL), v.1-2, 1941-58

Organic, Inorganic and Metal-Organic Compounds

SOLUBILITY RESOURCES (CALTECH LIBRARY)

<http://library.caltech.edu/collections/rpb/chemistry/chemistrysupp.htm#Solubility%20Resources>

CRYSTAL LATTICE STRUCTURES

<http://cst-www.nrl.navy.mil/lattice/index.html>

CAMBRIDGE STRUCTURAL DATABASE

Start Menu/Programs/CCDC → X Windows (ccdc@lib / 'cq' at prompt for ConQuest, or 'isostar' or 'isogen'. (if necessary, click 'next'...)

The Cambridge Structural Database (CSD) <http://www.ccdc.cam.ac.uk> contains structural information on over 250,000 carbon containing molecules (<1000 atoms), including organics, compounds of main group elements, organometallics and metal complexes. In this regard, the CSD is extremely valuable because Gmelin is not yet up to date with respect to all the literature of the 1980's and 1990's.

The CSD has recently increased the the size limit for polymeric compounds to no more than 24 residues. Higher oligomers are covered by the Protein Data Bank <http://www.rcsb.org/pdb/holdings.html>

The CSD contains the crystal structures of the major and minor amino acids and numerous small peptides, and has a very convenient way to search for structural characterized (non-protein) peptides according to their amino acid sequence.

The CSD covers mono-, di- and tri-nucleotides; higher oligomers are covered by the Nucleic Acids Database < <http://ndb-mirror-2.rutgers.edu/> >

The ICSD (Inorganic Crystal Structure Database) on STN and the PDB (Brookhaven Protein Data Bank) < <http://www.rcsb.org/pdb/index.html> > are complementary databases. The ICSD includes solid state inorganic compounds, such as simple salts, silicates, oxides, etc. Crystal structures of metals and metal alloys are covered by CRYSTMET[®] Structure and Powder Database for Metals and Intermetallic Compounds..(Toth).

The CSD reflects the published literature. It is fully retrospective and is updated on a current basis. All information is abstracted from primary journals and associated supplementary information in both hard-copy and electronic forms. The CSD is the official depository for crystal structure data for more than 50 journals.

Each CSD entry contains the following information:

- Bibliographic, textual and numerical information
- Chemical diagram
- Crystal structure data
- Filters (secondary search criteria)

Documentation and tutorials available at:

http://www.ccdc.cam.ac.uk/support/csd_doc/zdocmain.html

HAZARDOUS PROPERTIES DATA

TOXNET <http://www.nlm.nih.gov/pubs/factsheets/toxnetfs.html>

System of files related to toxicology, etc.

HSDB (HAZARDOUS SUBSTANCES DATABANK)

Extensive data on 4500 potentially hazardous chemicals. Fully referenced and peer-reviewed.

CHEM IDplus

Synonyms, structures, regulatory list information, and links to many other databases.

TOXLINE

Bibliographic database (3M citations) focused on drugs and chemicals

IRIS, CCRIS, GENE-TOX, DART/ETIC, TRI, NCI-3D

ACUTE TOXICITY DATABASE <http://www.cerc.usgs.gov/data/acute/acute.html>

Compound/Species data (e.g. LC-50 data for various exposures)

ENVIRONMENTAL FATE DATA BASE

<http://esc.syrres.com/efdb.htm>

MATERIAL SAFETY DATA SHEETS

<http://www.ilpi.com/msds/suppliers.html>

CALTECH CCE SAFETY MANUA

<http://chemistry.caltech.edu/resources/safety.html>

CALTECH ENVIRONMENTAL HEALTH AND SAFETY OFFICE

<http://safety.caltech.edu/home.htm>

CHEM LIST - (Regulated Chemicals Listing) - SciFinder Scholar Database

227,000 Chemical Substances on ... Chemical Inventories and Regulatory Lists

Bretherick's HANDBOOK OF REACTIVE CHEMICAL HAZARDS, 6 ed., v.1-2, 1999

SFL REF T55.3.H3 B73

DANGEROUS PROPERTIES OF INDUSTRIAL MATERIALS (SAX), 6th ed., 1984

SFL REF / MIL-8 REF T55.3.H3 S3

SIGMA-ALDRICH LIBRARY OF CHEMICAL SAFETY DATA, v.1-2, 1988

MIL-8 REF T55.3.H3 S54

REGISTRY OF TOXIC EFFECTS OF CHEMICAL COMPOUNDS, V.1-5, 1985/86

SFL REF RA1215 .R4

DOSE (DICTIONARY OF SUBSTANCES AND THEIR EFFECTS, v.1-7, 1992-

SFL REF RA1193 .D53

SYNTHETIC METHODS / COMMERCIAL AVAILABILITY

CHEMACX.COM <http://chemacx.cambridgesoft.com/chemacx/index.asp>

Comprehensive on-line catalog from over 210 chemical suppliers ... research community

CHEM SOURCES <http://db.chemsources.com/chemsources/>

200,000 chemical compounds from 7,200 companies. CAS RN for 100K and MF for 60K.

CHEM CATS - Commercially Available Chemicals - SciFinder Scholar Database

3.7 million records from 631 suppliers.

BEILSTEIN CROSSFIRE / SCIFINDER SCHOLAR (CAS React)

Structure searches can be limited to preparative reactions

ORGANIC SYNTHESSES ONLINE <http://www.orgsyn.org/>

Detailed experimental methods for the synthesis of organic compounds.

ORGANIC SYNTHESSES (PRINT) (V.1-77, Collective volumes 1-9)

MIL-8 REF QD 262 O7

INORGANIC SYNTHESSES, v.1-32, 1939+

Recent volumes ... coordination compounds, metal cluster & cyclopentadienyl complexes.

METHODS IN ORGANIC SYNTHESIS <http://www.rsc.org/is/database/moshome.htm>

Text searchable database covering important current developments (2000+).

NATURAL PRODUCT UPDATES <http://www.rsc.org/CFNPU/NPUsearchPage.cfm>

Text searchable database covering new developments in natural product chemistry (2000+).

e-EROS http://www3.interscience.wiley.com:8098/eros_about_fs.html

Online version of Paquette's Encyclopedia of Reagents for Organic Synthesis

ORGANIC REACTIONS, v. 1-59, 1942+

Book length articles on selected organic reactions MIL-8 REF QD251 O7

HOUBEN-WEYL - Methoden der Organischen Chemie, ~100 vols.

Detailed experimental procedures for the best methods (Text generally in German)

COMPREHENSIVE ORGANIC SYNTHESIS; Selectivity, strategy..., v.1-9, 1991

Carbon-Carbon bond forming, introduction of hetero-atoms and hetero-atom conversion.

COMP. ORGANIC FUNCTIONAL GROUP TRANSFORMATIONS. v.1-7, 1995

Introduction and interconversion of functional groups.

COMPREHENSIVE ORGANIC TRANSFORMATIONS (Larock). 1989, 2nd ed. 1999.

Organized according to the functional group being synthesized. 2nd. ed. is an update.