

Finding Chemistry Information

Chemistry:

Chemistry is the branch of physical science and research that deals with:

- elementary substances
- forms of matter [of which all bodies are composed],
- laws that regulate the combination of these elements
- various phenomena that impact on substances and matter

Chemistry is divided into two large subdivisions:

- 1) organic [pertaining to substances with carbon atoms]
- 2) inorganic [everything else]

General Search Methods:

1. Registry Numbers Searching

- Chemical Abstracts (CAS RN) has assigned a registry number (RN) to substances referred to in articles and papers being abstracted.

Note: a registry or RN number is always shown in brackets. e.g. [439-14-5]

So, how to find CAS Registry Numbers

- Catalogs (e.g. Aldrich)
- Merck Index
- Chem ID (can access through Toxline)

2. Other Searching Methods:

- Structure Searching
- Searching Chemical Names
- Molecular Formula (/MF)

Locate Related Information in Our Library:

1. Some Core Reference Items:

Title	Description	Call Number
CRC handbook of chemistry and physics	1) Tabulations of diverse chemical and physical properties. 2) Start here for physical data with minimal description	Reference QD65.C82 2000/01
Dictionary of Organic Compounds	The Dictionary provides a host of basic information about organic compounds including (often) a graphical representation of the structure and references to important publications.	Reference QD246 .D5 1996
The Merck Index	1) Brief entries on most common organic chemicals, especially those used in the chemical, biochemical, and pharmaceutical industries. 2) Excellent source for physical and physiological properties, common names, and CAS RN. 3) Entries point to more descriptive sources.	Reference RS51 .M4 1996

2. Databases:

Title	Coverage	CAS # Search
Beilstein Abstracts	Organic chemistry. Indexes the chemical literature and provides structure, property and reaction data.	No
Chemical Abstracts Service	All areas of chemistry (Librarian-mediated searching only)	Yes
Chemistry Preprint Server	All areas of chemistry — latest research in chemistry.	No

Medline	Chemical information relating to medical science, including pharmacology, biochemical and biotechnology.	Yes
Toxline	Information in all areas of toxicology, including chemicals and pharmaceuticals, pesticides, and environmental pollutants.	Yes

3. Internet Resources:

Name	Description
American Chemical Society http://www.acs.org/	This site provides information about ACS Publications, journals, topical issues, jobs, grants, continuing education, meetings, chemical history and events.
Chem ID plus http://chem.sis.nlm.nih.gov/chemidplus/cmplxqry.html	ChemIDplus is a free, web-based search system that provides access to structure and nomenclature authority files used for the identification of chemical substances cited in National Library of Medicine (NLM) databases. The database contains over 367,000 chemical records, of which over 142,000 include chemical structures, and is searchable by Name, Synonym, CAS Registry Number, Molecular Formula, Classification Code, Locator Code, and Structure
IUPAC Chemical Nomenclature: http://www.chem.qmw.ac.uk/iupac/ IUPAC Nomenclature of Organic Chemistry: http://www.acdlabs.com/iupac/nomenclature/	Two good nomenclature sites, easily browsable and searchable.
NIST Chemistry WebBook , http://webbook.nist.gov/chemistry/	The NIST Chemistry WebBook contains thermochemical data for over 6500 organic and small inorganic compounds, reaction thermochemistry data for over 9800 reactions, IR spectra for over 8700 compounds, mass spectra for over 12,600 compounds, electronic / vibrational spectra for over 4100 compounds, UV/VIS spectra for 400 compounds, constants of diatomic molecules (spectroscopic data) for over 600 compounds, ion energetics data for over 16,000 compounds, and thermophysical property data for 33 fluids. There are many avenues for searching the database. Structures are given for most species, as well as common and commercial names. [free]
PhysProp Database, http://esc.syrres.com/interkow/physdemo.htm	The Physical Properties Database contains names and physical properties for over 25,250 chemicals. Physical properties are collected from a wide variety of sources, and include experimental, extrapolated, and estimated values for melting point, boiling point, water solubility, octanol-water partition coefficient, vapor pressure, pKa, Henry's law constant, and OH rate constant in the atmosphere. The web demo version is searchable only by CAS registry number, and does not show chemical structures or full literature references. [demo 25,000 free. subscription]

4. Regional Resources:

- UC Berkeley Chemistry Library: <http://www.lib.berkeley.edu/CHEM/>
- Stanford University -- Swain Library of Chemistry and Chemical Engineering: <http://library.stanford.edu/depts/swain/>