

Internet resources for

# chemistry



**intute** : science, engineering & technology

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## The best of the Web

### Welcome to this guide to the best of the Web for Chemistry.

In these pages you will find a selection of some of the most useful websites for students, lecturers and researchers in Chemistry.

The selection is by no means exhaustive, but it should give you a flavour of the range of resources available on the Internet for chemistry.

## Supporting your Internet research

For those interested in exploring the wider Web, we offer free Internet search and training services for further and higher education via *Intute* – details of these can be found at the end of the guide.

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## Intute

This booklet is brought to you by *Intute*, a free Internet service providing you with access to the very best Web resources for education and research, evaluated and selected by a network of subject specialists.

[www.intute.ac.uk](http://www.intute.ac.uk)

## Expert advice

*Intute* services are developed in collaboration with staff from over seventy universities, colleges and research institutions across the UK – pooling expertise to share nationally.

Your guide for this booklet is:

**intute : science, engineering & technology**

– based at The University of Manchester and Heriot-Watt University.

*Intute* is funded by the Joint Information Systems Committee (JISC) with support from the ESRC and the Arts and Humanities Research Council (AHRC).

### Contact:

[www.intute.ac.uk/feedback.html](http://www.intute.ac.uk/feedback.html)

*Note: Intute was formerly known as the Resource Discovery Network (RDN). Intute: Science, Engineering & Technology comprises the former RDN hubs, EEVL, GEsources and PSigate.*

## Bibliographic databases

*For the majority of bibliographic databases access is restricted to institutional subscribers.*

### SciFinder Scholar

<http://www.cas.org/SCIFINDER/SCHOLAR/>

A major chemistry database maintained by the American Chemical Society. SciFinder Scholar is the world's largest collection of organic and inorganic substance information. The database covers more than 35 million substance records from the Chemical Abstracts Registry file, together with over 20 million abstracts from more than 9,500 journals, patents, conferences and reports in the CAPlus file. Users can search by author name, chemical substance or reaction, research topic or patent. *An institutional subscription is required for access.*

### CrossFire

<http://www.mimas.ac.uk/crossfire/>

CrossFire is one of the largest chemical databases in existence. Produced by MDL (formerly Beilstein), it features two primary components. The Beilstein Database covers organic chemistry, from 1771 to present, including information about structure, reactions, citations and physical property data. The database contains more than 8 million structures and 10 million reactions. The Beilstein Database also contains the Beilstein CrossFire Abstracts Database, which contains over 600,000 original author abstracts from 1980-present, and the EcoPharm database. The Gmelin database deals with inorganic and organometallic chemistry, and comprises more than 1.5 million compounds. Gmelin also contains information about materials, ceramics, glasses, alloys and minerals. This site contains details about subscriptions, registration, downloadable software, documentation, worked examples, news and other information about CrossFire. *An institutional subscription is required for access.*

### ISI Web of Knowledge

<http://wos.mimas.ac.uk/>

The Web of Knowledge service provides access to a number of databases in the sciences and other disciplines, including the Science Citation Index from 1981, ISI Proceedings Science and Technical edition from 1990, Current Contents Connect Physical, Chemical and Earth Sciences edition, Journal Citation Reports, ISI Chemistry, and Derwent Innovations Index. This platform provides a unique way of searching, including the ability to cross-search the content of multiple products and external resources simultaneously. *An institutional subscription is required for access.*

### Analytical Abstracts

<http://www.rsc.org/aa>

Analytical Abstracts is a major current awareness and information retrieval service for analytical scientists, published by the Royal Society of Chemistry. More than 100 international journals are scanned for inclusion. Around 1,400 abstracts are included in each monthly issue of the printed journal – allowing readers to scan the current worldwide analytical literature conveniently and rapidly. Subscribers to Analytical Abstracts receive the monthly printed journal. Subscribers may arrange free site-wide access to the fully searchable Analytical Abstracts Online (Analytical WebBase) which contains over one-third of a million records from 1980 to date, and is updated weekly. Topics covered include: chromatography, spectrometry, radiochemical methods, clinical and biochemical analysis, and radiochemical methods.

*An institutional subscription is required for access.*

### Chemical Database Service (CDS)

<http://cds.dl.ac.uk/cds/cds.html>

Based at the Daresbury Laboratory (UK), the Chemical Database Service (CDS) provides online access to a number of quality databases covering areas including spectroscopy, crystallography, organic and physical chemistry. The service is free to academics at UK universities. Support, training and advice are available via the website and also from dedicated helpdesks.

*Registration required for access.*

### Inspec

<http://edina.ac.uk/inspec/>

Published by the IEEE, Inspec is the leading English-language bibliographic information service providing access to the world's scientific and technical literature in physics, electrical engineering, electronics, communications, control engineering, computers, computing, information technology, manufacturing, production and mechanical engineering. The database also contains extensive information relevant to physical chemists.

*An institutional subscription is required for access.*

## Data collections and databanks

*These resources provide you with physical and chemical data, sometimes in a form that you can import.*

### DETERM Thermophysical Properties Database

<http://cds.dl.ac.uk/cds/datasets/physchem/determin/determin.html>

DETERM is part of the Chemical Database Service (CDS) based at the Daresbury Laboratory (UK). It provides information on the thermophysical properties of compounds and compound mixtures. It includes phase equilibrium data, excess properties, calorific properties, interfacial properties, transport properties, pressure volume temperature (PVT) data, electrolyte data, azeotropic data, identification of substances and bibliographic information. The database is accessed using a client on the user's PC. The required software and documentation can be downloaded through a link available at the website.

The service is free to academics at UK universities.

*Registration required for access.*

### ChemFinder.com

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

A site provided by CambridgeSoft which allows searching for any chemical by name, formula, CAS number, molecular weight, or by drawing a chemical structure or substructure. The information provided includes: physical properties, physical data, hazards, and online ordering. The site also includes links to related sites. Individual access to ChemFinder is complimentary on a limited basis. A more comprehensive commercial database is also available.

ChemFinder covers many fewer substances than Beilstein CrossFire, or SciFinder Scholar, but it covers the more commonly requested ones.

### NIST ChemistryWebBook

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

The NIST Chemistry WebBook, prepared by the US National Institute of Standards and Technology, provides users with access to chemical and physical property data for chemical species through the Internet. Data provided are from collections maintained by the NIST Standard Reference Data Program. Searching can be direct for chemical species, or indirect searches can be carried out based on related data. Varieties of searches can be undertaken: formulae, chemical names, CAS Registry numbers, ionisation energy, electron affinity, molecular weight, etc.

### **NDRL Radiation Chemistry Data Centre**

<http://allen.rad.nd.edu>

The Radiation Chemistry Data Centre at Notre Dame Radiation Laboratory hosts a series of databases covering kinetic, spectroscopic and thermodynamic data for processes in solution involving reactive intermediates (such as free radicals and excited states). The website contains databases of chemical property and kinetics information, listings of recent papers in radiation chemistry and photochemistry, and a bibliographic database.

### **Organic Syntheses Website and Database**

<http://www.orgsyn.org/>

A free fully-searchable database comprising over 80 years' worth of reaction information contained in the printed 'Organic Syntheses' journal, published by John Wiley and Sons, Inc. Users can draw compounds or reactions via the ChemDraw plug-in and combine these with a range of property and keyword information. In addition to the more advanced search, there is a simple Boolean search form which allows users to type in keywords.

### **WebElements™ Periodic Table**

<http://www.webelements.com/>

WebElements, by Dr Mark J Winter, aims to be a high quality source of information relating to the periodic table. Coverage is such that professional scientists and students at school will find something useful. The site contains thousands of graphics showing elements' structures and periodic properties. The site is available in two versions: a professional version and a scholar's version. A bulletin board is also available.

### **Chemcyclopedia**

<http://www.chemcyc.org/ME2/Default.asp>

A free database provided by the American Chemical Society (ACS), Chemcyclopedia is a catalogue of commercially-available compounds. It is searchable by company name, CAS registry number and category (chiral chemistry; drug discovery and development services; custom manufacturing and custom synthesis). If a category is chosen, users may also apply a filter to further streamline the search. The results provide a list of suppliers from which the chemicals may be purchased.

## Bilbao Crystallographic Server

<http://www.cryst.ehu.es>

This is the homepage of Bilbao Crystallographic Server, a collection of crystallographic programs and databases provided by the Materials Laboratory, University of Basque Country, Spain. It provides information about 230 space groups, generators and general positions, Wyckoff positions, maximal subgroups, and normalisers. It also provides information on space group representations, group-subgroup relations, and solid state applications.

## Fundamental Physical Constants

<http://physics.nist.gov/cuu/Constants/>

This database gives values of the basic constants and conversion factors of physics and chemistry resulting from the 2002 adjustment of the fundamental physical constants as published by the CODATA (Committee on Data for Science and Technology) Task Group on Fundamental Constants and recommended for international use by CODATA. Site content also includes: the latest conversion factors for energy equivalents recommended by CODATA for international use; a searchable bibliography containing about 2000 published papers on the constants and related precision measurements; an introduction to the constants for non-experts; and links to selected scientific data. This site is a service of the NIST (National Institute of Standards and Technology) Physics Laboratory.

# Journals

*A selection of websites useful for finding out about chemistry journals.*

## American Chemical Society Publications

<http://pubs.acs.org/about.html>

The American Chemical Society (ACS) publishes over 30 journals covering all aspects of chemistry. Their website offers access to contents lists and abstracts, subscription details and instructions for authors. Access to full text is available to subscribers or by purchase of individual articles. UK HE institutions can subscribe via the JISC funded site licence initiative (UK students should check with their University/College library whether access is available).

## RSC (Royal Society of Chemistry) Journals Archive

<http://www.rsc.org/Publishing/Journals/DigitalArchive/Index.asp>

The RSC Archive contains almost 1.4 million searchable pages of chemical science papers published by the Royal Society of Chemistry over 164 years (1841–2004) that can be leased or purchased outright. Content can be searched by year, author, abstract, journal or general text. UK HE can subscribe via a JISC agreement. (UK students should check with their University/College library whether access is available.)

## Alphabetical List of Chemistry Journals and Magazines

[http://www.rci.rutgers.edu/~longhu/ChemJournalList\\_Hu.html](http://www.rci.rutgers.edu/~longhu/ChemJournalList_Hu.html)

A list of links to chemistry journals and magazines, in alphabetical order, provided by Professor Longqin Hu, from Rutgers, the State University of New Jersey.

## Chemistry Journals

<http://www.ch.cam.ac.uk/c2k/cj/>

The Goodman Group at Cambridge University compiles and maintains this exhaustive list of chemistry and chemistry-related journals. Journals are listed by publisher, and each journal title points to either the full text of the journals, to tables of contents, or to supplementary material, as appropriate. Links are checked on a regular basis, and if a title is no longer available, the date of last connection is provided.

## Free Full-Text Journals in Chemistry

<http://www.abc.chemistry.bsu.by/current/fulltext.htm>

This site provides lists of full text chemistry journals which are either permanently or temporarily available free of charge. For each journal, a hyperlink is provided to the publisher's or journal's website and brief details of availability are provided. Maintained by Alexander Ragoisha of the Belarusian State University, the site is also available in Russian.

## Web directories

*A selection of sites that provide an insight into the range and quality of freely available web directories in chemistry.*

### Chemindustry.com: Worldwide Search Engine of the Chemical Industry

<http://www.chemindustry.com/>

ChemIndustry.com is a leading comprehensive directory and search engine for chemical and related industry professionals. The directory contains tens of thousands of chemical industry related entities and contains the full text of millions of pages. Specialised searches can be performed for chemical names, jobs, and consultants. The site is also available in Chinese, French and German.

## **CHEMINFO: Chemical Information Sources**

<http://www.indiana.edu/~cheminfo/>

CHEMINFO is a resource from Indiana University designed to help students find and learn how to use chemistry information resources on the Internet and elsewhere. It provides two resource guides: SIRCh (Selected Internet Resources for Chemistry) and CCIIM (Clearinghouse for Chemical Information Instructional Materials). Databases compiled or maintained at Indiana University, Bloomington, and other free databases on the Web can be searched. Full text chemical information course material is also available.

## **Links for Chemists: Chemistry Section of the WWW Virtual Library**

<http://www.liv.ac.uk/Chemistry/Links/links.html>

The chemistry section of the World Wide Web virtual library is compiled by the University of Liverpool, Department of Chemistry. The resources are placed in various categories including: university chemistry departments; companies and industrial links; chemical literature and publishing; general chemical information sites; employment links; organisations; software; general topics and other link sites. The site is available in English, German and French, with and without frames.

## **Martindale's Reference Desk: Virtual Chemistry Center**

<http://www.martindalecenter.com/GradChemistry.html>

This is a very extensive list of links to sites, compiled by Jim Martindale, covering the whole of chemistry, and including databases, courses and tutorials, books and journals, safety manuals, periodic tables and subject specific material.

## **Intute: Science, Engineering and Technology: Chemistry**

<http://www.intute.ac.uk/scienceandtechnology/chemistry/>

This resource contains approx. 4,200 descriptions of freely available Web-based high quality chemistry resources. The catalogue contains links to full text tutorials and lecture notes, to databases and databanks, journal websites, email lists, professional societies, reference material, etc. There is also a free science magazine Spotlight that discusses topical issues in science, and a chemistry timeline.

## **Organic Chemistry Resources Worldwide**

<http://www.organicworldwide.net/>

This website aims to collect and annotate synthetic organic chemistry sites. It is divided into six sections: part 1: literature: databases, articles, journals, patents, dissertations, etc; part 2: the bench: chemicals, solvents, safety, laboratory techniques, purification, and scientific instruments; part 3: structural analysis: NMR, mass spectrometry, infrared, UV/visible; part 4: the desk: synthesis planning, drawing, nomenclature, etc; part 5: communication: conferences, etc; part 6: additional activities. There is a subject index, and also a search facility.

## Professional societies, institutes and associations

*A selection of the key contact groups for chemistry worldwide.*

### Royal Society of Chemistry (RSC)

<http://www.rsc.org/>

The home page of the learned society for chemistry and the professional body for chemists in the United Kingdom. The site is divided into six main areas: publishing (journals, books, databases, etc); details of membership and member activities; education; science and technology (policy, awards, parliamentary activities); details of the society's library; and details of the society (structure, news, campaigns).

### Chemical Industries Association

<http://www.cia.org.uk/newsite/>

The UK Chemical Industries Association website provides a members only area and a general area. This latter includes: details of the association and its activities; information on the chemical industry and sustainability; a young person's network; educational resources; a bookshop; news releases; and other resources.

### International Union of Crystallography (IUCr)

<http://www.iucr.org/>

The IUCr aims to promote international cooperation in crystallography and to contribute to all aspects of crystallography, to promote international publication of crystallographic research, to facilitate standardisation of methods, units, nomenclatures and symbols, and to form a focus for the relations of crystallography to other sciences. Its website describes IUCr activities and provides access to: journals contents pages and abstracts; publications lists; a full text newsletter in PDF format; full text crystallography educational material; links to related sites; a world database of crystallographers; a history of crystallography; news; jobs; book reviews; CIF, the crystallographic information file (specification, dictionaries, software, documentation, current work, conferences); and mailing lists. There are several mirror sites.

### International Union of Pure and Applied Chemistry (IUPAC)

<http://www.iupac.org/>

IUPAC was formed in 1919 and seeks to advance the worldwide aspects of the chemical sciences and to contribute to the application of chemistry in the service of mankind. The IUPAC website gives details of IUPAC activities, together with educational materials; work on nomenclature and symbols; chemical elements; and publications (some available full text). Mirror sites are available.

## chemistry.org (The website of the American Chemical Society)

<http://www.chemistry.org/portal/a/c/s/1/home.html>

The website of the American Chemical Society (ACS) comprises a number of extensive sections: for professionals, for ACS members, for educators and students, policy makers, enthusiasts, and a personalised 'mychemistry.org' area. There are full text feature articles, information on databases and directories, educational sites, news and current awareness, and a range of member services.

## Mailing lists

*Mailing lists can be useful for exchanging information and for general current awareness in a specific field or topic. Below is a selection of useful lists in chemistry.*

### Chem-Education Mailing List

<http://www.jiscmail.ac.uk/lists/CHEM-EDUCATION.html>

The Chem-Education mailing list, hosted by JISCmail, covers a wide range of chemistry topics from the perspective of those involved in chemistry teaching, particularly in higher education. The list archive can be searched or browsed.

### Inorganic Chemistry Mailing List

<http://www.jiscmail.ac.uk/lists/INORGANIC-CHEMISTRY.html>

Hosted by JISCmail, this mailing list covers all aspects of inorganic chemistry. The list archive can be searched or browsed.

### ORGLIST: Organic Chemistry Mailing List

<http://www.orglist.net/>

ORGLIST is a mailing list for the discussion of organic chemistry, founded in 1997 and now comprising more than 700 members. Users can sign up free of charge for the list, and also search archives of all messages posted to date, searching by author, date, thread or subject. The list is not moderated.

### Computational Chemistry List (CCL)

<http://www.ccl.net/>

The Computational Chemistry List (CCL) is a mailing list for computational chemistry researchers to exchange information and experiences. All postings to this list are archived and available for downloading. It also archives other information and software useful to computational chemists.

## Educational resources

*There is a wide range of Web-based resources that support learning and teaching in chemistry.*

### Internet Chemist

<http://www.vts.intute.ac.uk/tutorial/chemistry>

This is one of a large set of tutorials from the Virtual Training Suite (VTS) of the Intute service. These tutorials are free, “teach yourself” online tools that let you practice and develop your Internet skills in specific subjects. Each tutorial has been created by subject specialists from universities and professional organisations across the UK.

### Chemguide: Helping You to Understand Chemistry

<http://www.chemguide.co.uk/>

Chemguide is a UK site, written by Jim Clark, aiming to cover parts of A-level or similar advanced chemistry courses that are often difficult for students to grasp. Topics include: atomic structure and bonding; inorganic chemistry; basic organic chemistry; organic reaction mechanisms; instrumental analysis and chemistry calculations.

### LearnNet

<http://www.chemsoc.org/networks/learnnet/>

LearnNet is an educational resource for chemistry teachers and students of all levels, produced by the Royal Society of Chemistry. The material in the database is classified in a number of ways – by subject, education level, and resource type. There is also a comprehensive list of careers resources, including interview skills and CV writing tips, resources which cover careers and events, magazines, journals, books (sections of some are available free online) and professional development. The site also includes other features, such as an exam doctor, discussion group, and sophisticated search tools.

### Named Reactions in Organic Chemistry

<http://orgchem.chem.uconn.edu/namereact/named.html>

This site provides details of over ninety named organic chemical reactions. The site provides primary bibliographic references, recent examples, and reaction equations and formulae. The site is provided by Professor Michael Smith, Chemistry Department, University of Connecticut.

## **Chemistry Hypermedia Project (CHP)**

<http://www.chem.vt.edu/chem-ed/index.html>

Developed and maintained at Virginia Tech's Department of Chemistry, CHP is a set of online resources for students, educators and scientists. Covering general chemistry, analytical chemistry, and analytical instrumentation, the resource contains a large collection of descriptions, definitions and examples in chemistry fundamentals.

## **Intute: Science, Engineering and Technology: Chemistry**

<http://www.intute.ac.uk/sciences/chemistry/>

Incorporating the PSIGate Physical Sciences chemistry gateway, this resource comprises a fully searchable catalogue of approx 4,200 resource descriptions in chemistry. All the resources are full text and freely accessible, and have been selected by subject specialists. The catalogue contains hundreds of full text tutorials and lecture notes.

## **Introductory University Chemistry Course 1**

<http://www.intute.ac.uk/sciences/reference/plambeck/chem1/ua101.html>

This resource comprises a full text online set of tutorials, originally prepared by Jim Plambeck of the University of Alberta. Part 1 offers 34 separate tutorials primarily in physical and inorganic chemistry.

## **Introductory University Chemistry Course 2**

<http://www.intute.ac.uk/sciences/reference/plambeck/chem2/ua102.html>

This resource comprises a full text online set of tutorials, originally prepared by Jim Plambeck of the University of Alberta. Part 2 offers 37 separate tutorials primarily in physical and inorganic chemistry.

## Chemical nomenclature

*Some guides on the naming of chemical compounds.*

### **Nomenclature Lite: a Guide to Naming and Indexing Chemical Compounds**

<http://php.indiana.edu/~davisc/Contents.htm>

This website describes the general rules for naming and indexing chemical compounds. The site is provided by Charles H Davis of Indiana University.

### **IUPAC Compendium of Chemical Terminology (Gold Book)**

<http://www.chemsoc.org/chembytes/goldbook/>

This is an online version of the IUPAC Compendium of Chemical Terminology (2nd edition, 1997). Nearly 7000 terms covering the whole of chemistry are included in this version, with definitions supplied by international experts and approved by IUPAC. The online version also includes definitions from ISO and the 'International Vocabulary of Basic and General Terms in Metrology'. Users may search by keywords or free text phrases. Adobe Acrobat Reader is required to view the document itself.

### **IUPAC Nomenclature**

<http://www.chem.qmul.ac.uk/iupac/>

Based at Queen Mary University of London, this site hosts a series of online guides to chemical nomenclature prepared by the International Union of Pure and Applied Chemistry (IUPAC) and the International Union of Biochemistry and Molecular Biology (IUBMB). These guides provide a comprehensive resource for the naming of organic chemical compounds.

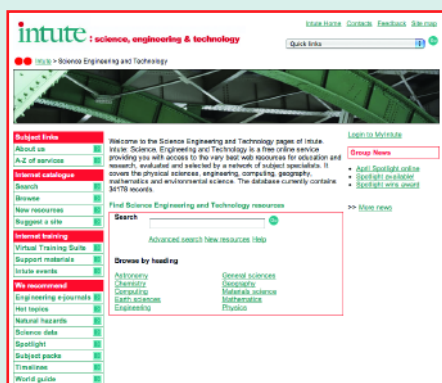
## Discover the best of the Web using Intute

The Internet can be a powerful tool for learning, teaching and research, offering a huge range of resources and services. However, finding relevant information online can be a daunting task, and issues of trust, quality and poor search skills are very real and significant concerns – particularly in education and research contexts.

*Intute* exists to help students, teachers, researchers and librarians make sense of the Web by providing access to the very best Internet resources for education and research, selected and evaluated by a network of subject specialists.

### intute : science, engineering & technology

- The **Internet catalogue** provides access to thousands of high-quality Internet resources, selected and described by subject specialists, and covers all key areas of the physical sciences, geography, engineering, mathematics and computing.
- The **Virtual Training Suite** offers free Internet training with a set of “teach-yourself” online tutorials, designed to help students develop their Internet research skills.
- Free **support materials** for universities and colleges, such as flyers, posters, leaflets and presentations as well as a range of “best of the Web” subject booklets.
- **Recommended subject services** – such as **The World Guide** comprising guides to over 270 countries, interactive maps, thousands of satellite images, etc.; **Ejournal Search Engine (EJSE)** with access to over 250 freely available full-text ejournals relevant to engineering, mathematics and computing; the **Spotlight Magazine** providing a growing database of unique articles on current topics in science; and thematic **Timelines** containing dozens of key events which have shaped the world as we know it, together with suggested *Intute* searches for further research.



## Getting involved with Intute

- Sign up for a personal **MyIntute** account, which provides weekly email updates of recently added websites and allows you to save resources of interest.
- **Working with Intute.** Join our community of users of online resources by suggesting sites for the database or embedding *Intute* services in your own websites and Virtual Learning Environments using our sophisticated **MyIntute Include** services.

[www.intute.ac.uk](http://www.intute.ac.uk)

Contact: [www.intute.ac.uk/feedback.html](http://www.intute.ac.uk/feedback.html)

