

Using the World-Wide Computer Network, Internet, in Chemical Sciences

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Modern computer and information technology has opened up many possibilities for communicating various types of information efficiently throughout the world. A non-technical introduction to some of the available resources on the computer network, Internet, is given in this paper. Hints on where to start exploring the Internet and how to obtain information are provided. Methods for communicating between scientists, how to access archives, and modern multi-media information systems are described. Several examples of services available to chemists are shown.

Computers and information technology have made their way into all scientific disciplines, including chemistry.¹ Computers are used for many tasks, e.g. word processing, data acquisition, data plotting, data analysis, statistics, communication, simulations and visualization. The fast growth and massive production of knowledge in science demand rapid and efficient ways of retrieving,^{2,3} and communicating, information. Both the United States of America and the European Union⁴ have taken initiatives to establish electronic information highways. The most important electronic information highway today is the Internet, a world-wide computer network.

This paper describes some of the services available on the Internet, and in particular some of the services available to chemists.^{5,6} A non-technical introduction to some of the available Internet resources is provided, to get new users started, and hopefully new information is given to those who already use some of the services. The basic infrastructure necessary for using these services and resources is most often maintained by the computer centre or similar resource at the user's institution. Complete lists of services are not provided, merely some hints on which types of services are currently available, together with some pointers to where to start exploring the constantly evolving world of Internet.^{7–9} Quite often a particular Internet service is available by several methods, and not all methods available will be mentioned for the services listed here. The computer programs which are needed to use these services are available for a number of computer systems.

Many of the services offered to scientists are maintained by volunteers (e.g. other scientists), and often in their spare time. Therefore, the quality and availability of the services may be variable, depending on the time the maintainers can spare for the service. However, Internet

services are highly collaborative and if one thinks a service is no good, one should improve it by contributing to it. All users of the Internet should be aware of the network etiquette, also called netiquette.^{10,11}

Rapid person-to-person communication can be achieved by electronic mail, and the Internet offers several methods for reaching a large number of persons, and taking part in 'electronic' scientific discussions with persons all over the world. In addition, various services exist that enable scientists to retrieve information and computer programs, search databases and exchange information. One of the advantages of Internet services is that the services are accessible to many people, and that new information is almost instantly available. However, the large amount of information is a problem on the Internet just as in printed matter. Several Internet services currently available to chemists are described in the following sections.

General technicalities

It should be noted that since the services described in this paper are accessible from a large number of different types of computer systems with a large number of different programs, all information herein may not be appropriate for all users. Because of the large number of different computer programs available for accessing the same Internet service, the author has chosen to describe the Internet resources in general terms and has not assumed that a particular computer system or computer program is being used.

Each computer on the network has a unique address, the Internet address. This address is a sequence of dot-separated numbers, e.g. 128.214.248.6. Each computer also has a symbolic address, in this case the symbolic

address corresponding to the numeric address above is nic.funet.fi. The symbolic address has the general form: machine.domain.country. From the above symbolic address we can see that the computer *nic* is located in domain *funet* in Finland. The symbolic address is the most persistent address and should be used if possible. The numeric address of a computer may change, but the symbolic address may still be the same. However, some computer systems require the numeric form.

A fundamental notion of modern computer technology is the client-server model. Simply stated, the computer program you use to retrieve information from the network is the client. The client is served by a server, which is a remote computer (or the one on your desk) with available information and a computer program running to take care of the exchange of information and data between the client and the server.

The Internet is an open network, and as such vulnerable to inappropriate activities, e.g. unauthorized access to data. There are many advantages of using Internet; however, one should be conscious about having a reasonable level of protection against inappropriate activities. For most users this is simply to make sure that passwords are changed frequently, that the passwords are difficult to guess, and that the passwords are kept secret.

By participating in Internet communication and using information systems, one will leave a trace in log-files kept on the servers. Also, messages one has communicated several years ago can be retrieved from some archive server and be referenced later. This is really no different from scientific publication in journals, so one should keep in mind that messages communicated on the Internet are public statements.

Communicating with other scientists

Electronic mail. One common way of person-to-person communication is by means of electronic mail. The communication is fast and the recipient can read the message when time allows, in contrast to telephone communication. This is particularly advantageous for communication between scientists living in very different time zones. In order to use electronic mail one must have a setup of infrastructure, typically handled by the computer centre or equivalent. The user also needs a mail program on his/her computer to be able to send and receive mail.

There exist a large number of different mail programs on most computer systems, and with different user interfaces. However, all mail programs require that the user enter the address of the recipient and often a subject heading. The electronic mail address of the author is edvard@fagmed.uit.no, i.e. the name of the recipient followed by the @ character and then a symbolic address of the computer which should receive the message.

Electronic mail users should take care to create meaningful subject headings. Many people receive a lot of electronic mail every day, and need to select messages by looking at the subject headings. Person-to-person electronic mail is useful for communicating textual information. It is possible to communicate binary data, e.g. computer programs, but this requires additional software and coding at the sender side and similar software and decoding on the recipient side.¹²

Mailing list servers. Another useful way of communication is person-to-group communication. One method for doing this is by use of a list server. One person volunteers to create and maintain the necessary software to enable the use of a list server. Those who are interested in participating in such a list send an electronic mail message to the list server maintainer with a request to be added to the list of participants (Table 1). Note that mailing list servers have two addresses, one for administrative purposes (e.g. subscription) and one for communicating with the other participants. Messages sent to the list are distributed to all participants, and administrative messages are read by the list administrator or are processed automatically by a computer program. Some mailing lists are moderated, i.e. one or more volunteers read the incoming messages and judge the content for its suitability for distribution to all participants. On other list servers only digests are distributed. Unmoderated and moderated list servers may handle highly specialized scientific discussions.

The address of the mailing list is similar to a personal electronic mail address, and should be used when communicating messages to the list. The method of registration, however, varies from list to list, and you should consult mailing list compilations available on the Internet for details on which lists are available and how to register and participate.^{13,14} The author has taken the effort to make sure that the mailing list servers in Table 1 are reachable by the instructions given. Unfortunately the

Table 1. Examples of electronic mail discussion lists of interest to chemists.^a

Administrative address	Topic	Subscription request
LISTSERV@PDB.PDB.BNL.GOV	Protein DataBank discussions	subscribe PDB-L your name
LISTSERV@UWF.CC.UWF.EDU	Chemistry education	sub CHEMED-L your name
CHEMISTRY-REQUEST@OSC.EDU	Computational chemistry	name, affiliation and electronic mail address
LISTERV@IUBVM.UCS.INDIANA.EDU	Chemical information sources	sub CHMINF-L your name
ORGREQ@EXTREME.CHEM.RPI.EDU	Organic chemistry	sub ORGCHEM-L your name

^a Subscription requests should be entered as a one-line message, and not as a subject. When registered by the list server one receives detailed information on how to participate in the discussion and how to cancel one's subscription to the list.

compilations of mailing list servers available on the Internet^{13,14} seem to have some inaccuracies, probably due to the dynamic nature of the Internet. Compilations of chemistry-related electronic mailing lists have also been published in the literature.^{3,15}

News. A better organized but somewhat similar system is called News (also called NetNews and USENET News). News is organized into hierarchic interest groups (Table 2). For electronic mail the user needs a mail reader as client software, while for News there is a need for another type of client software, the News-reader. Such software exist for most modern computer systems. Many News-readers also have the capability to post (send a message) to News groups, or one needs a separate computer program for that purpose. It is similar to electronic mail, but the recipient is the name of the News group. As for electronic mail messages, users should be conscious about the subject heading and be concise and accurate in the message text. By using the News client software the user can join any News group available. The infrastructure for News is maintained by the computer centre or similar, and not all possible News groups are available at all institutions. By using the News system one can get answers to problems and discuss advanced topics with participants from all over the world. It is really similar to participate in electronic mailing lists. Each user can read and respond to the News messages whenever time permits. Many interest groups are available both as list servers and as News groups, so that participants can use the most convenient or practical way of communicating, and all users see the same messages either in the electronic mailbox or in the News group.

A very nice feature of many News groups is that volunteers maintain documents with frequently asked questions (FAQs) and answers, so that the discussions in the News groups will be on new topics and not ones discussed or answered many times before. It is a good habit to check the FAQ of a News group before posting a question. FAQs and other useful information are archived at rtfm.mit.edu [18.181.0.24] (see below and Fig. 1). New users should use the News groups news.announce.newus-

```
ftp rtfm.mit.edu
Connected to BLOOM-PICAYUNE.MIT.EDU.
220 rtfm ftpd (wu-2.4(24) with built-in ls); bugs to
ftp-bugs@rtfm.mit.edu
Name (rtfm.mit.edu:edvard): anonymous
331 Guest login ok, send your complete e-mail address as password.
Password: edvard@fagmed.uit.no
230 Guest login ok, access restrictions apply.
ftp> cd /pub/usenet/news.answers/www/faq
250 CWD command successful.
ftp> dir
200 PORT command successful.
150 Opening ASCII mode data connection for /bin/ls.
total61
-rw-r-- 22 root 3 36213 Aug 26 00:37 part1
-rw-rw-r-- 22 root 3 24775 Aug 26 00:37 part2
226 Transfer complete.
134 bytes received in 0.0078 seconds (17 Kbytes/s)
ftp> get part1
200 PORT command successful.
150 Opening ASCII mode data connection for part1 (36213 bytes).
226 Transfer complete.
local: part1 remote: part1
37016 bytes received in 8.8 seconds (4.1 Kbytes/s)
ftp> get part2
200 PORT command successful.
150 Opening ASCII mode data connection for part2 (24775 bytes).
226 Transfer complete.
local: part2 remote: part2
25338 bytes received in 5.6 seconds (4.5 Kbytes/s)
ftp> bye
221 Goodbye.
```

Fig. 1. A sample anonymous ftp session. The commands entered by the user are shown in bold type. The electronic mail address given as password will not be visible on the screen. This session demonstrates how to obtain documents archived at rtfm.mit.edu [18.181.0.24], and a few of the commands available with ftp. For more details on available commands, users should read the documentation of the client software in use.

ers (explanatory postings to new users) and news.newusers.questions (questions and answers for new users) to make themselves familiar with the service.

Information systems

A large number of computers throughout the world have computer programs and information of general interest

Table 2. News groups related to chemistry.^a

Group name	Topic
alt.drugs.chemistry	Drug chemistry and synthesis
bionet.journals.contents	Table of contents of many scientific journals
bionet.molec-model	Physical and chemical aspects of molecular modelling
bionet.xtallography	Protein crystallography
sci.chem	Chemistry and related sciences
sci.chem.electrochem	Electrochemistry
sci.chem.labware	Laboratory equipment
sci.engr.biomed	Biomedical engineering
sci.engr.chem	Chemical engineering
sci.polymers	Polymer science
sci.techniques.mag-resonance	Magnetic resonance imaging and spectroscopy

^a In addition to these groups, national chemistry News groups may exist, e.g. in Norway there is a chemistry News group called no.kjemi.

available. The most popular archives have identical copies several places in the world (mirror sites) to save the Internet from overloading. One should always use the nearest archive if possible, and avoid massive file transfer in the peak hours at the server site.

Accessing file archives with ftp. One method of accessing such archives is by using a client program called ftp (file transfer protocol) or similar. Many archive servers have a setup which allows users restricted access without the use of a secret password. Such setup is known as 'anonymous ftp'. When you want to contact an archive site you must start the ftp computer program and indicate either the numeric or symbolic address of the archive server. You will be asked for a user name, which should be anonymous (hence the name anonymous ftp), and then a password, which should be your electronic mail address (Fig. 1). Archive servers often store the electronic mail addresses of the users for statistics. Some servers will not grant access unless a valid electronic mail address has been entered as password. When all this has been done, you have a limited set of operations³ you can perform on the archive (Fig. 1). Compilations of available anonymous ftp sites of general interest¹⁶ and of interest to chemists¹⁷ are available on the Internet.

Often the archives are hierarchically organized in a directory named pub, for public. The archives are often organized in several sub-directories, e.g. by software category or computer system type. If you want to contribute software or information to such site, the most common place is in a directory called incoming. One should carefully read the instructions available at most sites before donating data to such archive. The incoming directory is often configured such that the users can not see what is stored there. It is up to the maintainer of the archive to move the new information to the appropriate place in the file hierarchy or delete it if it is not considered suitable for the archive. New users should also read instructions archived at the various sites, often in files named README or similar.

Accessing file archives and services with electronic mail. Some people do not have access to ftp, and for this and other reasons several archives can be accessed using electronic mail.¹⁷ Users access the archive by sending a message to the archive by using the electronic mail address

of the archive (Table 3). The message is often one or more commands from a limited set of available commands for retrieving help, obtaining a listing of available information and retrieving computer programs and information resources. When computer programs are retrieved, it is often necessary to code binary information into data which the mailing system can handle. The recipient then needs a computer program for decoding the information into binary data.¹² Instructions on how to obtain decoding software and how to use it are normally obtained from the file archive, often by sending the message **help** by electronic mail to the archive mail server. Then one will most likely obtain general instructions on how to use the archive, and this is usually a good method for learning how to use a new archive site by electronic mail.

A useful service accessible by electronic mail is run by the publisher Springer. A large number of journals have their tables of contents distributed by electronic mail. You can subscribe to this service and receive the table of contents of the journals of interest as soon as they are available, often a couple of weeks before shipping of the printed journal from the publisher. Send the message **help** to svjps@vax.ntp.springer.de to obtain information on how to use this service. For a small fee, you can also receive abstracts in your electronic mailbox. The journal tables of contents are also distributed to the News group bionet.journals.contents¹⁸ (Table 2), which also contains a number of other journal tables of contents.

Accessing archives and information using gopher. A more sophisticated method of accessing remote file archives is by using a system called gopher. In many cases the necessary client program is also called gopher. Gopher presents a menu-based interface to the archive, and is an easy to use interface to archives of computer programs and information (Table 4). By starting the available gopher client you will see the default menu, typically one set up by the computer centre at your institution. If you want to direct the client to a particular server you will have to inform the client software about the address of the server, e.g. by appending the address on the command line. The exact method of informing the client software about the gopher server one wants to contact may vary from client to client. A useful gopher server is that run by The American Chemical Society, which can be contacted by entering the command `gopher acsinfo.acs.org` (or `gopher`

Table 3. Archives reachable by anonymous ftp and by electronic mail.^a

Address of archive	Directory	Description	Mail server address
nic.funet.fi [128.214.6.100]	/pub/sci/chem	Chemistry archives, computer programs and various	mailserver@ftp.funet.fi
osc.edu [128.146.36.5]	/pub/chemistry	Computational Chemistry Mailing List (CCL) Archives	mailserv@osc.edu
ftp.pdb.bnl.gov [130.199.144.1]		Brookhaven National Laboratory, the Protein DataBank	
physics.arizona.edu [128.196.188.8]	/afc	Buckminsterfullerene bibliography	

^a Send the message **help** to the mail server address to obtain instructions on how to use electronic mail for retrieval.

Table 4. Gopher servers related to chemistry.^a

Address of server	Description
acsinfo.acs.org [134.243.230.66]	The American Chemical Society
atlas.chem.utah.edu [128.110.196.10]	Material Safety Data Sheets
infx.infor.com [198.136.167.1]	Book catalog
slvaxa.umsl.edu [134.124.1.1]	Chemistry textbooks in print
jcp.uchicago.edu [128.135.44.113]	J. Chem. Phys. Preprints, JCP Express
gopher.pdb.bnl.gov [130.199.144.1]	Brookhaven National Laboratory, the Protein DataBank
infomeister.osc.edu [128.146.36.5]	Computational Chemistry Mailing List (CCL) Archives (port 73)
ftp.uci.edu [128.200.80.20]	Material from the journal Protein Science (port 1071)
jchemed.chem.wisc.edu [144.92.90.150]	Journal of Chemical Education
gopher.genethon.fr [192.70.45.2]	Back issues of journal table of contents
gopher.iucr.ac.uk [192.70.242.1]	The International Union of Crystallography

^a Port numbers are not listed unless they are different from default.

134.243.230.66), assuming that the client program is called gopher and that the proper method of specifying a server is on the command line. Sometimes one also needs to specify a port number, e.g. gopher acsinfo.acs.org 70. Since 70 is the default port number for gopher, it can be omitted from the command. However, not all gopher servers use the default port number. Some gopher sites of potential interest are listed in Table 4. A more complete listing is available by anonymous ftp.^{16,17}

Multimedia on the network. The most recent and sophisticated information system available on the Internet is called the World-Wide Web^{19,20} or WWW or simply 'the Web'. In this system ftp, gopher and several other existing information systems are embedded, such that existing archives can be utilized with this new technology. The Web has capabilities for combining text, graphics, sound and video into a complete multimedia environment, and may be considered as one large database with information stored around the world. Among the many advantages of this system is the nice user interface which makes it easy for novices to explore the world of Internet. There exist both character-based and graphics-based client software for the Web, and obviously the latter is preferred. As with gopher, Web documents can be linked to each other so that a multi-page document may be stored on several servers around the world, and yet appear to the user as one document. When using graphics based computer systems, the users simply point and click to obtain information. The information can be organized in clickable menus, clickable words in a text or clickable pictures. Different areas of a picture (e.g. a geographic map) can be linked to different types of information. Fill-in forms are available as interfaces to, e.g., searches in databases.

One of the most popular client programs for the Web (often called browsers) is called Mosaic, and is available for a number of computer systems.²¹ If you consider using the Web it is important to obtain the list of Frequently Asked Questions (FAQ)²¹ to read the basic information on how to get started, and explanations on technical details.

Unfortunately we need to delve somewhat more into

technical details to be able to understand what is going on when using the Web, and what the information source specifications mean (Table 5). When we point and click on Web documents we really do not need to know this technical information, but for new users it is important to know about it to get started. Each Web document has its own 'address' called a Uniform Resource Locator (URL),²¹ which is similar to a symbolic address, but is appended by a directory and file name, and prepended by the name of the transfer method used by the server. The transfer method may be, e.g., gopher or http, which is the Web method for transferring data. To direct the client to a certain document, the URL of the document may be entered on the command line (or by another appropriate method depending on the client software), e.g. mosaic http://atf1.fagmed.uit.no/mgl.html, which will retrieve information from the laboratory of the author.

Multimedia possibilities on the Internet open up many possibilities for enhanced exchange of information and data in chemistry, e.g. electronic publishing.^{22,23} It is possible to have a publication on the Internet where, e.g., the molecular structure of a compound is drawn in a figure. By clicking on the figure, a helper program for viewing three-dimensional molecular structures is started on your computer and the coordinates of the molecule are sent to your computer and drawn by the helper program.²⁴ By using the helper program you can rotate, render and view a three-dimensional image of the molecule as you wish, which is not restricted to the projection and rendering chosen by the authors of a publication in a printed journal. Helper programs need to be obtained and installed separately from the Web client software. Currently there are few pure electronic journals available,²⁵ although some efforts have been made towards electronic publishing in chemistry.^{22,23} Some Web-sites of potential interest to chemists are listed in Table 5.²⁶

Concluding Remarks

The biological scientific community has a large number of users of Internet resources, and many useful services exist to aid biological research. The chemistry community also

Table 5. World Wide Web servers related to chemistry.

Uniform resource locator	Description
http://www.chem.ucla.edu/chempointers.html	The official Chemistry Directory Service on the Web. Chemistry departments and services.
http://www2.shef.ac.uk/chemistry/chemistry-www-sites.html	Another directory of chemistry Web sites and services.
http://hackberry.chem.niu.edu:70/0/webpage.html	Chemistry on the Internet. Chemistry resources.
http://www.iucr.ac.uk/welcome.html	The International Union of Crystallography.
http://www.unige.ch/crystal/crystal_index.html	Crystallography directory service.
http://csd.vx2.ccdc.cam.ac.uk/	The Cambridge Crystallographic Data Centre. On-line software manuals.
http://www.csc.fi/lul/csc_chem.html	Chemistry at Centre for Scientific Computing (CSC) in Finland.
http://www2.shef.ac.uk/chemistry/web-elements/web-elements-home.html	Web Elements. Periodic table, isotope pattern calculator and element percentage calculator.
http://www.osc.edu/chemistry.html	Computational Chemistry Mailing List (CCL) Archives.
http://www.nih.gov/molecular_modelling/mmhome.html	Molecular modelling information and resources. A molecular modelling primer.
http://www.pdb.bnl.gov/	The Brookhaven National Laboratory Protein Databank (PDB).
http://www.gdb.org/Dan/proteins/nrl3d.html	Search for secondary structure elements in data from PDB.
http://www.nih.gov/htbin/pdb	Full text search of data from PDB.
http://ibc.wustl.edu/klotho/	Three-dimensional structures of biochemical compounds.
http://info.cas.org/welcome.html	Chemical Abstracts Services product information.

needs to utilize the efficient and valuable communication medium provided by the Internet. With such user-friendly systems as gopher and the Web, new users have easy access to the network resources, and added value is provided for established users. With the possibilities of multimedia on the Internet, many opportunities open up, and of particular interest is electronic publishing with a large increase in the value of the information provided. New users are encouraged to start using the Web, as this gives easy access to Internet resources. Chemists on the Internet may find it useful to at least have access to electronic mail and the Web. These systems may be useful in modern research activities. With the enormous potential and impact of electronic communication it is important that chemists use and take part in development of such services. The national chemical societies may consider initiating activities related to international networks and network resources to increase the knowledge of and use of this technology in all aspects of chemistry. In the future, the availability of electronic information, and the use of computer technology and appropriate software, may enable easier selection of relevant information, and may provide scientists with far more detailed information and data than before.

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- chem. Recently, a compilation of mailing lists has become available by WWW on <http://www.clark.net/pub/listserv/lb101.html>.
14. A compilation of chemistry-related mailing lists is available by gopher from [192.153.156.15] by choosing InterNIC Information Services (General Atomics) → Internet Resources → Chemistry Mailing Lists on the menus or by WWW as <gopher://is.internic.net/11/infoguide/resources/chemistry>.
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 16. A compilation of anonymous ftp sites is available from rtfm.mit.edu [18.181.0.24] in /pub/usenet/news.answers/ftp-list/sitelist. Note that the list is split in several parts.
 17. A compilation of various sites of potential interest to chemists is available from leon.nraps-ariadne-t.gr [143.233.2.1] in directory /pub/chemistry/sites.chem.
 18. Journals related to chemistry: *Biol. Chem.*, *J. Biol. Chem.*, *Clin. Chem.*, *Protein Sci.*, *Eur. J. Biochem.*
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 24. Helper programs for viewing molecular structures are e.g. XMOl and RasMol. More information about these helper programs and their use can be obtained by WWW on http://www.ch.ic.ac.uk/chemical_mime.html and on http://www.ch.ic.ac.uk/rzepa/RSC/CC/4_02963A.html.
 25. A list of available peer-reviewed electronic journals and related information can be obtained by WWW on <http://golgi.harvard.edu/journals.html>.
 26. By using WWW, all electronic documents referenced are available as supplementary material. Clickable menus corresponding to Tables 2–5 are available, as well as other sites of potential interest to chemists that have not been mentioned in this paper. The supplementary material is available by WWW only on <http://atf1.fagmed.uit.no/chemsuppl.html>.

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