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Author(s)	KOH THIAM SENG
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Surfing the World Wide Web for Chemistry Resources: An Introductory Tutorial

KOH THIAM SENG

Introduction

The World Wide Web (WWW) is the most recent hypertext information service to arrive on the Internet. In a hypertext information system, the reader may browse items of information in a non-sequential manner. This browsing is done by looking up predefined associative links between documents containing related information. The items of information that may be linked in the WWW documents or files include texts, pictures, sound clips and video clips.

Through surfing or navigating the Internet via the WWW, teachers and students are able to access relevant and timely information on practically any subject on a global basis. To access this information, they only need a computer system that is connected to the Internet and relevant software for browsing the WWW.

In this article, I have provided some basic information for chemistry teachers and students on how to get started on surfing the WWW and the types of chemical information and resources available on the Internet. It is not within the scope of this short article to explain the technical details for connecting a computer system to the Internet or to load the relevant software. For such information, the reader should consult the computer guru or expert in their respective work place.

Hardware and Software for Browsing the WWW

If you are planning to use the computer in the school to access the WWW, there is a good chance that your workplace computer is already connected to the Internet. You can easily check this with your computer network administrator or the teacher in charge of the computer systems in your school. However, to get your home computer connected to the Internet in Singapore, you will need a modem and a telephone line; preferably a dedicated line. You will also need to sign up with one of the local Internet service providers, either **Singnet** or **Pacific Internet** for an Internet account. From 1996 onwards, you will have a choice of signing up with the third Internet service provider, **Cyberway**. In order to enjoy full multimedia browsing, you will need to opt for Point-to-point Protocol (PPP) [or at least Serial Line Internet Protocol (SLIP)] for your connection to the Internet. PPP or SLIP connect your computer directly to the Internet while you are online.

There are a number of software available in the market for reading or browsing the documents or files on the WWW. Some of the more common browsers that may be installed into your computer include NSCA **Mosaic**, Netscape **Navigator**, TradeWave **WinWeb**, InterCon **NetShark Lite** and **Cello** (see the Appendix for the WWW sites where you may download these WWW browsers). In this article, the browsing of the WWW for chemistry resources will be illustrated using Netscape **Navigator** Version 1.22 running under Windows 3.1 on an IBM compatible PC.

Home Page

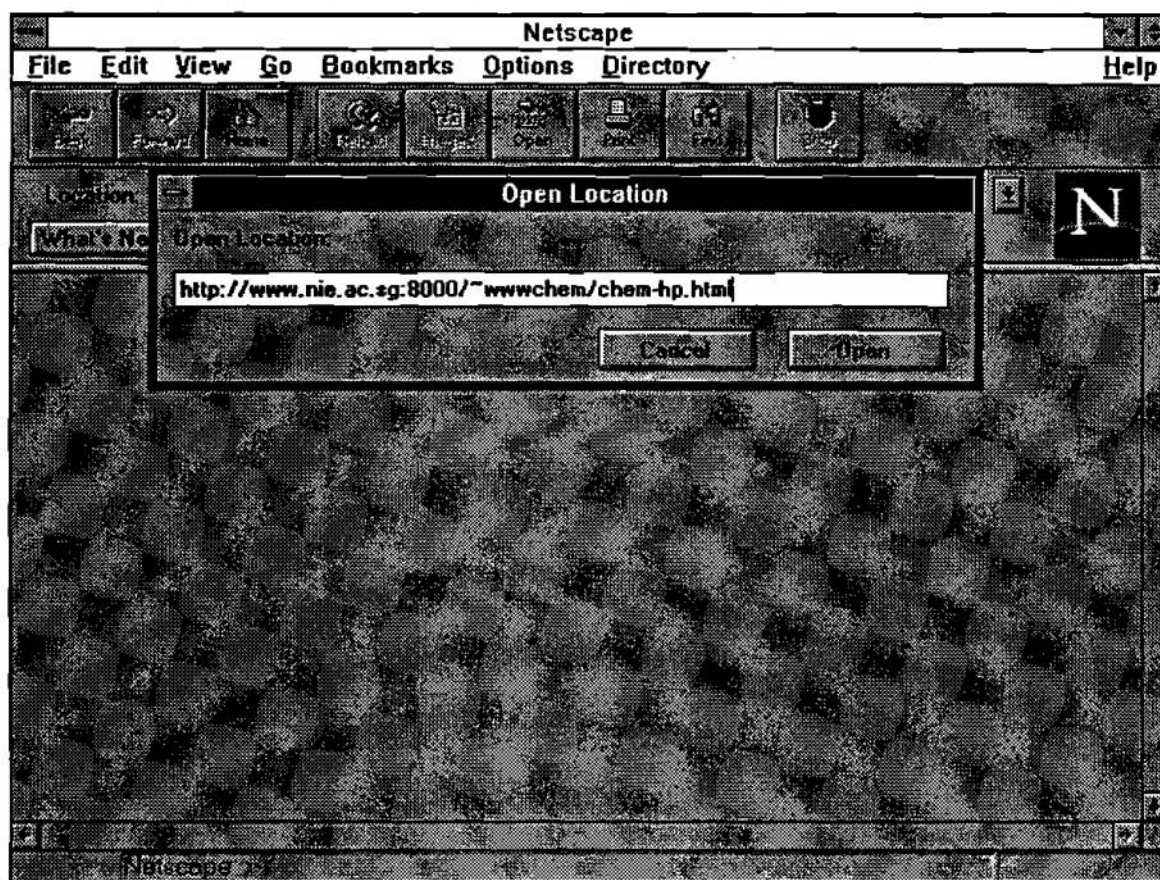
In order to start your browsing of the WWW, you need to access a suitable WWW home page i.e. a suitable starting document or file that contain predefined associative links to the information or resources that you require. In Singapore, for information and resources related to Chemistry, the home page that you could start at is the one created by the Division of Chemistry, National Institute of Education. The URL (uniform resource locator) or the internet "address" of this home page is

<http://www.nie.ac.sg:8000/~wwwchem/chem-hp.html>

The above URL may be entered into your browser using the following procedure. From the respective menu of the browser, select **FILE**. Under the **FILE** menu, select the item, **OPEN LOCATION** or **OPEN URL**. In the dialogue box obtained, enter the above URL without leaving any blank spaces in between and press the [ENTER] key or select the [OPEN] or [OK] button. It is important that the tilde sign, '~' is entered correctly. This sign is typically found on the extreme top left hand key of the main keyboard; just below the [ESC] key and above the [TAB] key. Generally, if you are using a mouse, selecting a particular menu or a menu item require you to move the mouse pointer or cursor (usually an arrow or a blinking line) over the menu or menu item and click the left mouse button once. A typical screen showing the dialogue box for entering the URL is depicted in Figure 1.

Figure 1

Entering the URL for NIE chemistry home page

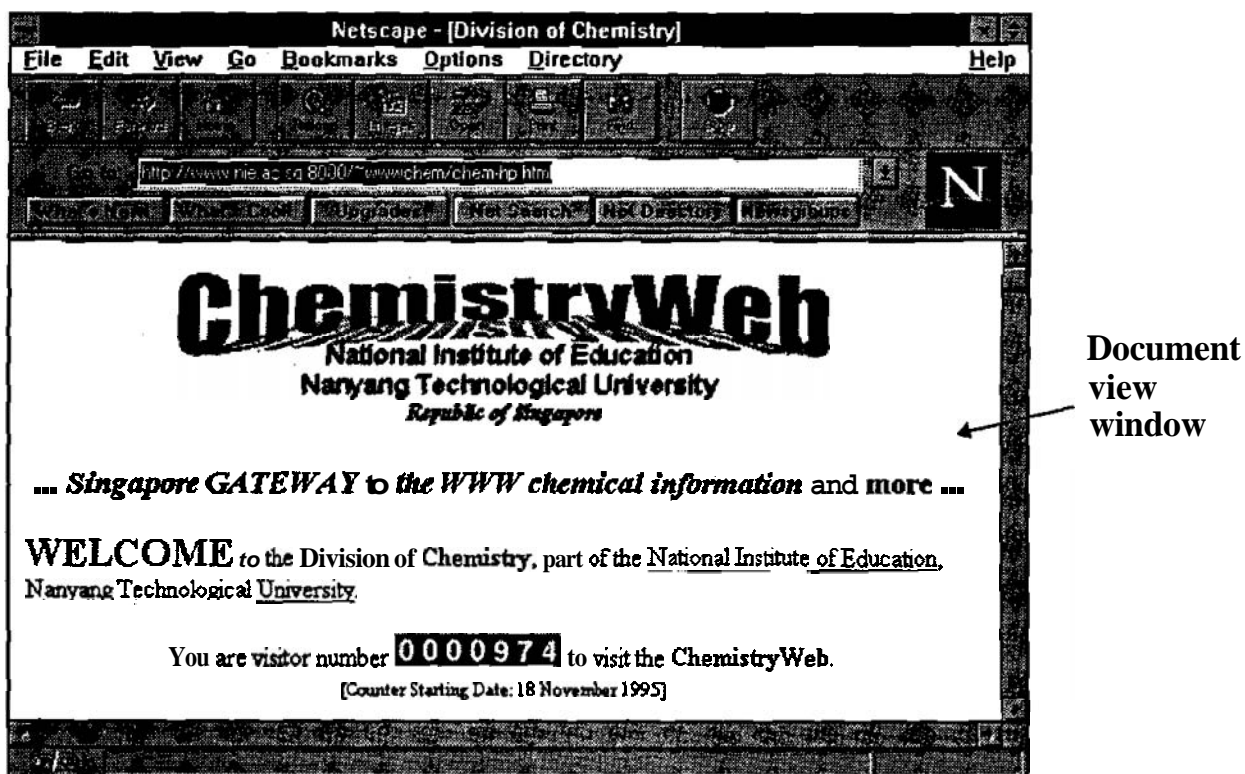


Navigating the WWW

Once the connection to the chemistry home page is made, the typical screen obtained is as depicted in Figure 2. If you are able to get connected to this chemistry home page at NIE, the rest is easy. You will be surfing the WWW in no time. You merely need to use the mouse to click on the various links that interest you. These links are easily identified. Text links comprise a single keyword or a phrase and are underlined and, by default, are coloured blue or pink. Graphic or iconic links have a bold blue or pink outline. For example, in Figure 2, the text links are National Institute of Education and Nanyang Technological University. If you want to access these links to obtain more information on these instructions, just use the mouse to click on any part of the phrase to get connected to the next document containing the detailed information required.

Figure 2

Top part of the NIE chemistry home page

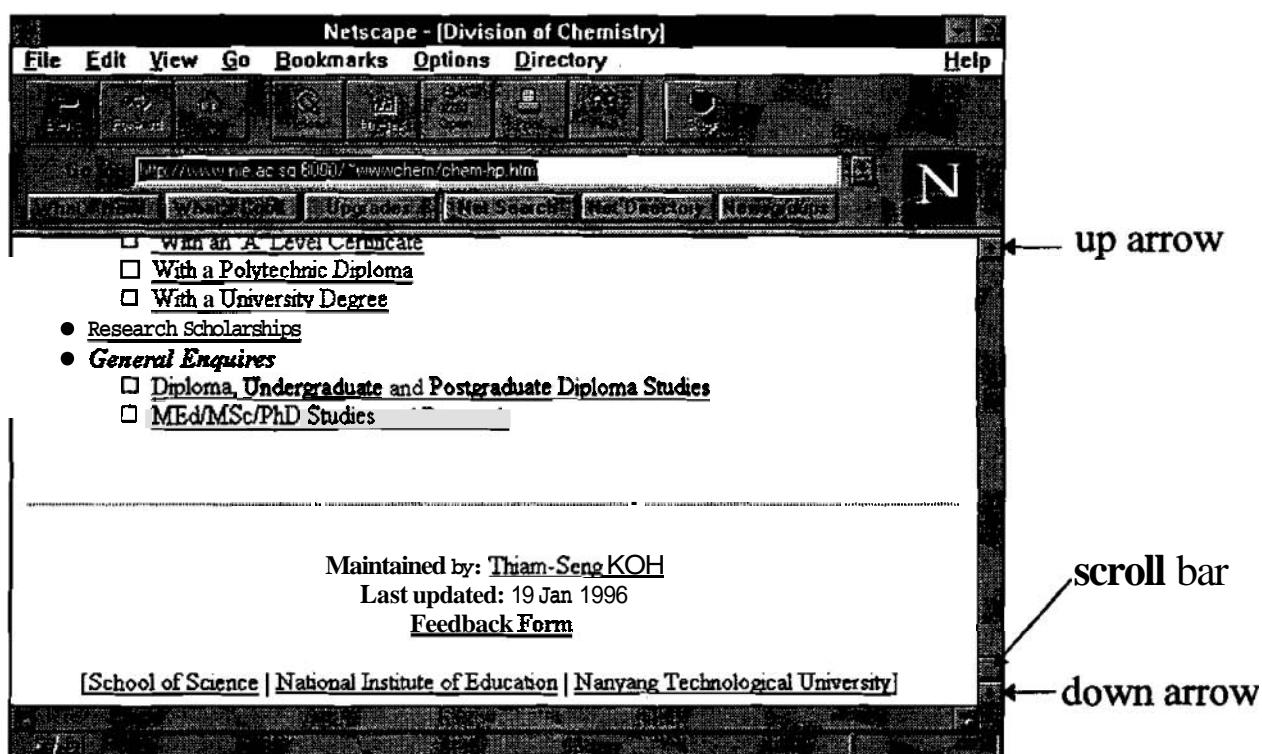


When you first access the home page, you will see the screen depicted in Figure 2. If the document is longer than could be shown in the document view window, as it is the case of the home page, you will need to use the mouse to move the scroll bar (see Figure 3) at the right hand side of the window. When the scroll bar is moved all the way down, you will see the bottom part of the document in the document view window as depicted in Figure 3. The scroll bar may be moved in a number of ways.

- You may move the mouse pointer or cursor over the up arrow or down arrow and click on it. Each click of the left button of the mouse will move a line of text up or down respectively.
- You may move the mouse pointer or cursor to any position above or below the scroll bar and click on it. Each click of the left button of the mouse will move the text up or down a window page.
- You may move the mouse pointer or cursor over the scroll bar and while holding down the left button of the mouse, you can drag the scroll bar up or down to move up or down the document very quickly.

Figure 3

Bottom part of NIE chemistry home page



It is important to remember that you can only see a window page of a document at a time. If the length of the document exceed this document view window (see Figure 2), you will need to use the scroll bar to see the remainder of the document. However, if the document falls within the document view window, an attempt to move the scroll bar will not lead to a change in the screen display.

Chemical Information and Resources on the WWW

In the course of your surfing the WWW, you will encounter the following types of resources on chemistry, namely,

- on-line documents on chemistry related topics
- demonstration software, freeware and shareware on chemistry
- discussion groups on chemistry related topics
- searching engines
- on-line courses and conferences.

For access to some of the links to the information and resources outlined above, see the Appendix attached. These links provided in the appendix are also found by browsing the chemistry home page. *However, it is important to note that much of the information that is found on the WWW is not peer refereed before it is deposited on the Web. You should critically review the information that you retrieve from the Web.*

On-line documents

A wide variety of on-line documents on chemistry for teaching and research may be retrieved from the WWW. Many university chemistry departments around the world provide up-to-date information on their faculty research and teaching. The number of chemistry departments around the world which maintain WWW sites is well over 300. The wealth of information maintained on these sites is particularly useful to career guidance counsellors and Singapore students who

intend to enrol in chemistry at an overseas university. The relevant information can now be accessed from their computers either at home or in school at a click of a button.

Teachers could retrieve sample lesson plans for chemistry and other teaching resources at different levels of schooling. Both teachers and students can get access to general information on many specialised topics in chemistry such as quantum and computational chemistry. On-line reference materials accessible at the click of the mouse button include the EPA toxicological data on a wide range of substances, periodic tables and on-line journals such as *Journal of Chemical Education: Software*.

Chemistry Software

A wide range of chemistry related software is available on the WWW for downloading onto your local computer from some remote computer system elsewhere in the world. These software packages include demonstration software of commercial packages, shareware and freeware. Demonstration software may either be merely software demonstrating all the features found in the software product or an actual functioning software with important features such as printing and/or copying across applications being disabled. Shareware are generally fully functioning software that may be copied for the purpose of evaluation. Typically, you may use shareware for up to 30 days to evaluate their usefulness and suitability. If you are satisfied with these software and want to continue to use them after the evaluation period, you are expected to register the use of these software with their respective authors and pay a specified sum. On the other hand, freeware, as the name suggests, are free and may be copied freely and used without making any payment to the authors.

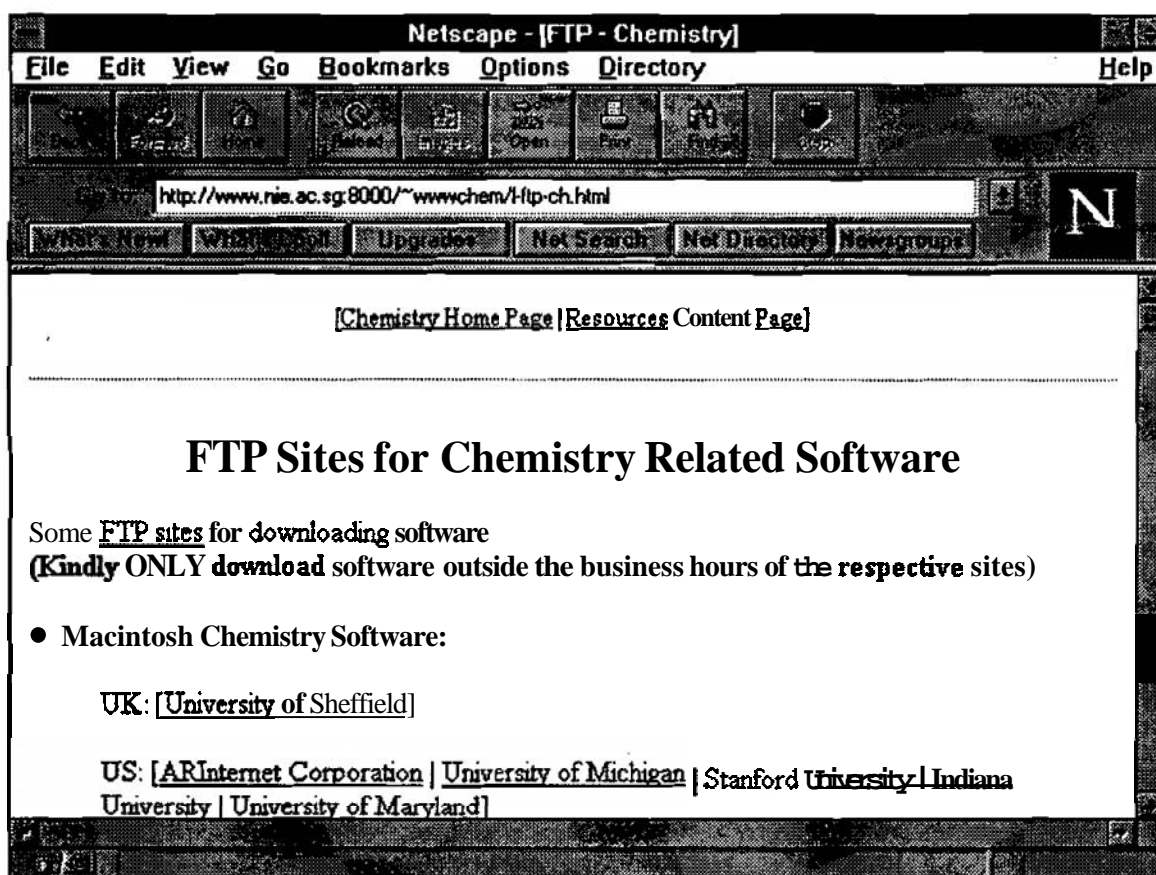
These chemistry related software may be downloaded via the web browser using FTP (file transfer protocol). FTP is a method of transferring files between remote computers. The types of files that may be transferred between computers include computer programs, text or document files, graphic, sound and video files. Many of the program files placed on these FTP sites are compressed files i.e. the original files have been compressed to reduce their sizes to speed

up their transfer across the computer network. One very common type of compressed file is the zip file i.e. files ending with the 'zip' extension, for example, 'orgtut.zip'. Once these zip files are downloaded or transferred to your computer, you will need to unzip or decompress them before using them. A common program for decompressing zip files is **winzip** (see the Appendix for the site to download the program).

In order to access some of these FTP sites around the world, click on the links provided in the chemistry home page under FTP sites. At the time of writing, links to some FTP sites are found in the document accessible from the link, Gateway to Chemistry Resources on the INTERNET in the chemistry home page. Once the connection to the latter link is made, the screen depicted in Figure 4 showing some FTP sites is seen by selecting the link, Chemistry related FTP sites.

Figure 4

Links to some FTP sites



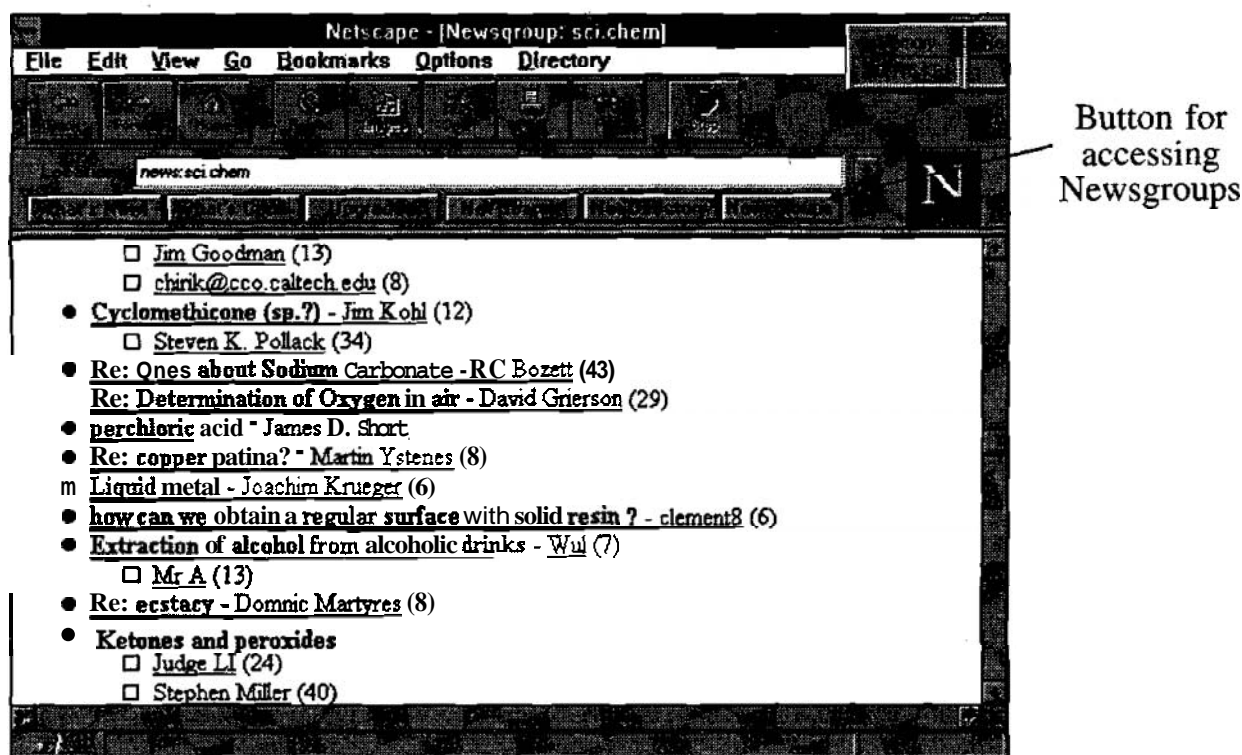
A good FTP site to visit is the one at CTI (Computers in Teaching Initiative) Centre for Chemistry at the University of Liverpool. The Centre maintains a catalogue of chemistry related software in addition to demonstration-software, shareware and freeware that may be downloaded to your computer. The 4th edition of the former catalogue provides detailed information on 427 chemistry related software. The details captured in the latter database include the price, the authors and publishers, the platform (Mac, IBM, etc.) for the software, the intended audience or users, a short description of the software and references to literature reviews of these software.

Discussion groups on chemistry related topics

There are discussion groups called USENET newsgroups that allow the users to exchange information with one another on the Internet on a broad range of topics which include chemistry related topics via the email. Some of the relevant newsgroups to chemistry teachers and students include **sci.chem**, **sci.edu**, **sci.chem.analytical**, **sci.chem.organomet** and **sci.polymers**. For example, if a teacher has some questions pertaining to general chemistry, then, he or she may wish to post or email the question to the **sci.chem** newsgroup to get the answers. However, if the teacher has some questions pertaining to analytical chemistry or polymer chemistry, then, he or she may post the question to the **sci.chem.analytical** and **sci.polymers** newsgroups respectively for the answers. These newsgroups may be accessed using the WWW browser.

Figure 5

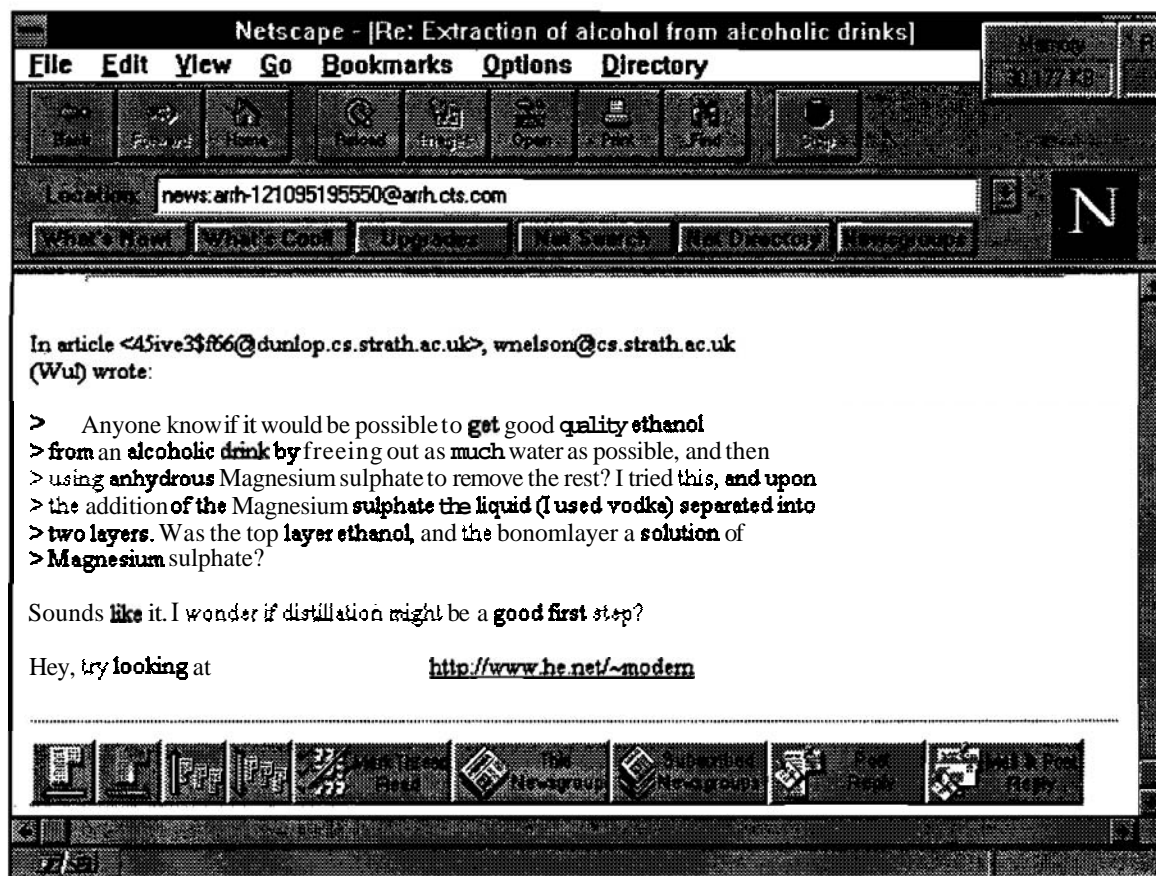
A directory of the sci.chem newsgroup



In Netscape **Navigator**, these newsgroups are accessible through clicking the [newsgroup] button as shown in Figure 5 assuming that the WWW browser is already configured to an appropriate news server (a computer system that stored the news items) and you have subscribed to these newsgroups. Some of the questions and replies posted on the **sci.chem** newsgroup are shown in Figure 5. Those news items in the directory that start with 'Re:', for example, 'Re: Determination of Oxygen in air' is the reply to a question posted to the newsgroup. In Figure 6, a reply to the question on the extraction of alcohol from alcoholic drinks is shown as an illustration.

Figure 6

A sample reply to a question posted on **sci.chem** newsgroup

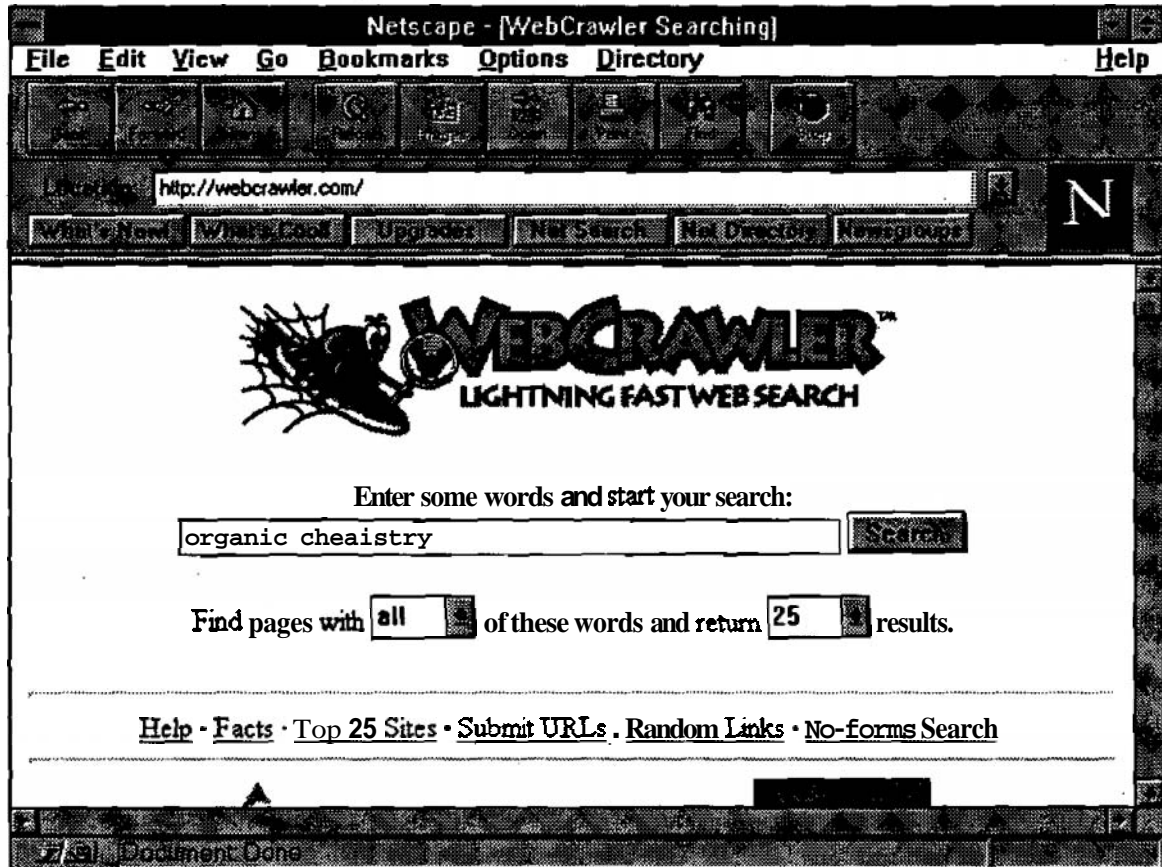


Search Engines

There are a range of tools or engines available on the WWW for the searching of chemistry related information by keywords. The home page of one searching tool, Webcrawler, is shown in Figure 7 (see the Appendix for the URL of some of these sites).

Figure 7

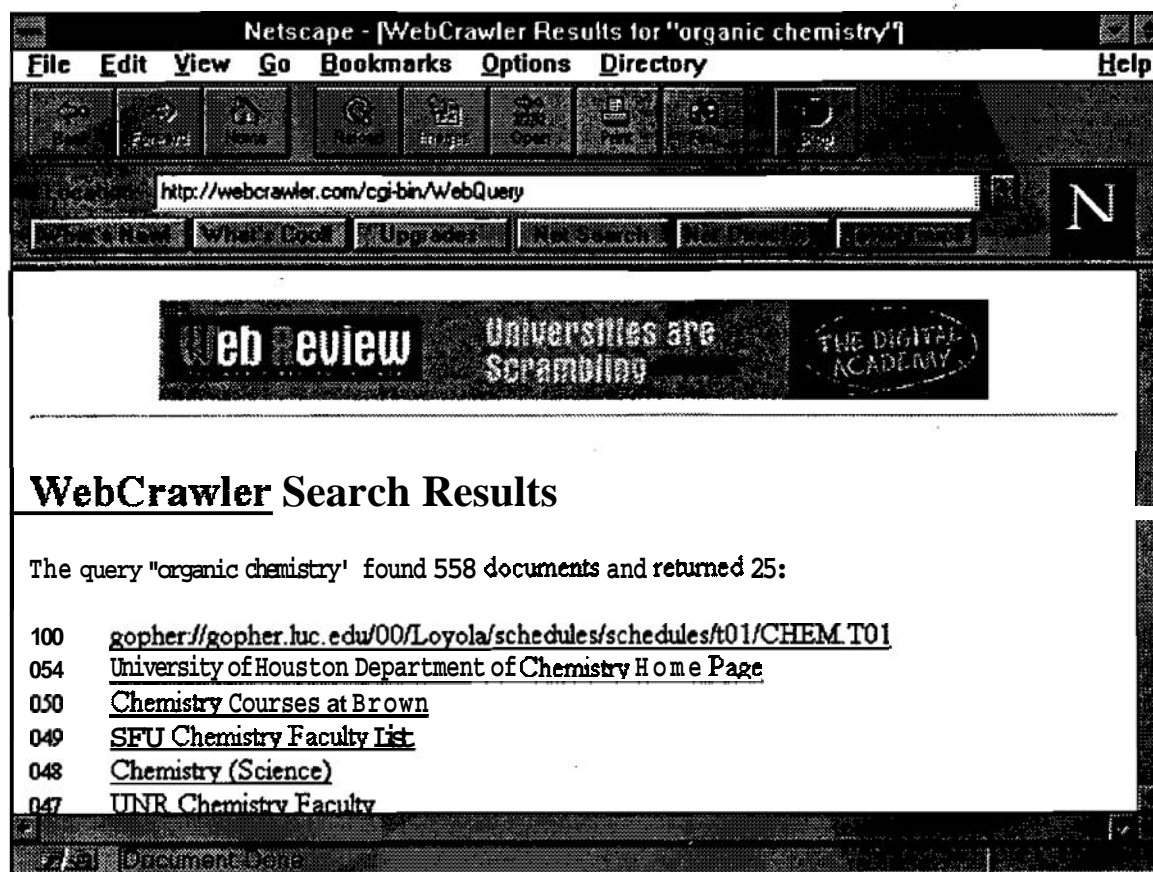
The home page of search tool, Webcrawler



Once the connection to the Webcrawler home page is made, the searching process is easily accomplished by typing in the keyword or keywords and clicking the [Search] (or [Submit]) button. The searching tool will then display the results by listing the Internet sites that contain the documents or files that include the keyword or keywords entered. For example, the query, 'organic chemistry' returned a result of 558 documents that contained the former keywords. The initial part of the result of the search is depicted in Figure 8.

Figure 8

A sample of the result on the query, 'organic chemistry' using Webcrawler



These search engines are useful to teachers and students who are interested in a fairly comprehensive search of resources on the Internet on a particular chemistry topic. They provide a convenient route for researching a particular area of chemistry for project work or for teaching a particular chemistry topic. The resources obtained on a particular topic from these searches generally complement and in some cases, supplement the information found in the libraries. However, as the search results obtained are dependent on the scope of the databases of the respective searching engines, it is important to use several search engines if a complete search of nearly all the available resources on a particular topic is required.

On-Line Courses and Conferences

Increasingly, the WWW has been used as a platform for on-line courses and conferences. These courses and conferences are announced on the WWW from time to time. The WWW browser is used to view the lessons for the course or the paper presented at the on-line conference. The participants interact with one another and the instructor or the authors via email. In 1995, there were several chemistry related courses and conferences conducted. They include a course on "Computational Chemistry for Chemical Educators" conducted by North Carolina Supercomputing Centre (NCSC) (<http://www.mcnc.org/HTML/ITD/NCSC/ccsyllabus.html>), an undergraduate course unit on environmental chemistry sponsored by the American Chemical Society (<http://dirac.py.iup.edu/college/chemistry/chem-course/webpage.html>) and the First Electronic Organic Chemistry Conference (<http://www.ch.ic.ac.uWectoc/>).

Some Concluding Remarks

The WWW is an extensive global source of educational resources that is open to exploration and application by chemistry teachers and students. In order to discover the richness of the resources available on the WWW, the reader has to start investing some time in browsing the WWW. Hopefully, this short article has provided sufficient information to get started on surfing the WWW and generated enough interest to do so. So, happy exploring. If you should encounter any problem surfing the chemical net, you may contact the author via email at kohts@nievax.nie.ac.sg.

Suggested Readings

1. Krol, E. *The Whole Internet: User's Guide and Catalog* (2nd Ed.). O'Reilly & Associates: Sebastopol, California, 1994.
2. Randall, N. *Teach Yourself the Internet: Around the World in 21 Days* (2nd Ed.). SAMS: Indianapolis, 1995.

3. Rzepa, H. S., Whitaker, B. J., Winter, M.J. Chemical Applications of the World-Wide-Web System. *Journal of the Chemical Society: Chemical Communications*, (1994) 1907-1910.
4. Heller, S. R. Analytical Chemistry Resources on the Internet. *Trends in Analytical Chemistry*, **13** (1994) 7-12.
5. Noble, D. Analyzing on the Internet. *Analytical Chemistry*, **67** (1995) 255A-259A.
6. Winter, M. J., Rzepa, H. S., Whitaker, J. Surfing the Chemical Net. *Chemistry in Britain*, **31** (1995) 685-689.
7. Krieger, J. H. Chemistry Sites Proliferate on the Internet's World Wide Web. *Chemical and Engineering News*, November 13 (1995) 35-46.
8. Bachrach, S. M. Electronic Conferencing on the Internet: The First Electronic Computational Chemistry Conference. *Journal of Chemical Information and Computer Sciences*, **35** (1995) 431-441.
9. Bachrach, S. M. (Ed.) *The Internet: A Guide for Chemists*. American Chemical Society, Washington DC, 1996.

APPENDIX: World Wide Web sites for chemistry and selected resources.

World Wide Web Browsers

NSCA Mosaic

ftp://ftp.ncsa.uiuc.edu/Web/Mosaic/Windows/Win31_x/mosaic20.exe

Netscape Navigator

<ftp://ftp5.netscape.com/2.0beta/windows/n16e20bl.exe>

At the time of writing, the above FTP site contains version 2.0 (beta) of the Navigator browser. This beta version is not fully tested yet and may contain some bugs.

TradeWave WinWeb

<ftp://ftp.einet.neVeineVpc/winweb/wwl1eval.exe>

InterCon NetShark Lite

<ftp://netshark.inter.neUpub/netshark/netshark.exe>

Cello

<ftp://ftp.law.cornell.edu/pub/LII/Cello/cello.zip>

Some WWW sites containing chemistry related materials

WWW Chemistry Catalogue:

<http://www.chem.ucla.edu/chempointers.html>

This site, which is maintained by Max Kopelevich (Department of Chemistry and Biochemistry, University of California Los Angeles), contains useful information on chemistry departments at universities around the world, chemistry related organisations such as chemical societies and a host of other goodies. The universities are listed by countries. A definite **MUST** for a visit. The general contents of the site is listed below:

- WWW Chemistry Sites at Academic Institutions
- WWW Chemistry Sites at Non-profit Organizations
- WWW Chemistry Sites at Commercial Organizations
- Other Lists of Chemistry Resources and Related WWW Virtual Libraries
- Some Chemistry Gopher Servers
- Some Chemistry FTP Servers
- Chemistry and Biochemistry USENET News Groups

Sheffield ChemDex: Chemistry Resources on the INTERNET

<http://www.shef.ac.uk/~chem/chemdex/>

This site, which provides HTTP pointers to chemical information and resources that are as extensive as those listed on the WWW Chemistry Catalogue, is maintained by Mark J. Winter (Sheffield University, UK). The listings include: universities (by country), chemistry related commercial organisations (by country), learned societies, USENET newsgroups, electronic journals, software packages, anonymous FTP sites, GOPHER sites, Listserv services, telnet services, etc.

LaTrobe WebChemistry

<http://www-chem.harvard.edu/webchem.html>

This site also provides HTTP pointers to chemical information and resources that are as extensive as those listed on the WWW Chemistry Catalogue and ChemDex. This listing is maintained by Joey Santos (La Trobe University, AUSTRALIA). The listings include: chemistry departments at universities (by country), anonymous FTP sites, chemistry gopher servers, chemistry databases and software, chemical Companies, on-line chemical information services, chemical publications and journals, USENET newsgroups, etc.

ChemEd: Chemistry Education Resources:

<http://hrvww-hpcc.astro.washington.edu/scied/chemistry.html>

Another good site to visit that offers a wide range of HTTP pointers to chemistry resources. This site is maintained by Alan Cairns (University of Washington, Seattle). The listings include: chemistry courses and hypertext documents, reference materials, curriculum materials (lesson plans, labs, etc.), images and databases, history of chemistry, FTP sites, etc.

Chemistry Teacher Resources:

<http://rampages.onramp.net/~jaldr/chemtchr.html>

This site, which is maintained by James Aldrich, caters specifically to chemistry teachers teaching at upper secondary and pre-university level.

Internet Resources for Chemistry:

<http://ww.inform.umd.edu:8080/UMS+State/UMD-Projects/MCTP/Technology/Chemistry.html>

This site, which is maintained by Professor Tom O' Haver (Department of Chemistry and Biochemistry, The University of Maryland), provides an index under the following headings: organisations, on-line conferences, on-line presentations, education, chemistry software, other chemistry resources on the internet, data, commercial, miscellaneous and discussion groups (listserv lists and newsgroup).

Some Chemistry Resources on the Internet:

<http://www.rpi.edu/dept/chem/cheminfo/chemres.html>

The pointers on this index are compiled by Gary Wiggins (Indiana University Chemistry Library) and maintained by Joseph Warden (Department of Chemistry, Rensselaer Polytechnic Institute). Headings used in this index are: book catalogues; databases; document delivery; email servers, list-servs, newsgroups, etc.; FTP resources; Gophers; guides to Internet resources; on-line search services; periodicals and conference proceedings (full text); periodicals and other documents (current awareness); software (including users groups); teaching resources; world-wide web resources; corporate web resources.

Chemistry Education Resources (Stony Brook):

<http://sbchem.sunysb.edu/cheedres.html>

Yet another site offering links to chemistry resources that are grouped under headings such as catalogues of chemistry education resources, computing and software links and ethics in science.

YAHOO Chemistry

<http://www.yahoo.com/Science/Chemistry/>

Index based on Yahoo search on chemistry.

Some FTP Sites For Chemistry And General Software

Singapore FTP sites for general software:

- a. Nanyang Technological University: **<ftp://ftp.ntu.ac.sg/>**
- b. National University of Singapore: **<ftp://ftp.nus.sg/>**

* The winzip program (**winzip56.exe**) may be downloaded from either the NUS or the NTU site. Once the connection to the site is made, click on the directories in the sequence given: /pub/windows/util/ for the NUS site and /pub/win3/util for the NTU site to download **winzip56.exe**.

Macintosh chemistry software:

- a. University of Sheffield: **<ftp://ftp.shef.ac.uk/pub/uni/academic/A-C/chem>**
- b. University of Michigan: **<ftp://archive.umich.edu/mac.misc/chemistry/>**
- c. Stanford University: **<ftp://sumex-aim.stanford.edu/mac/misc/chemistry/>**
- d. Indiana University: **<ftp://fly.bio.indiana.edu/chemistry/mac/>**
- e. University of Maryland: **<ftp://info.umd.edu/info/Computers/Macintosh/Math-Science/Chemistry/>**
- f. ARInternet Corporation: **<ftp://ftp.ari.net/pub/MacSciTech>**

DOS and Windows chemistry software:

- a. Simon Fraser University: **<ftp://ftpserver.sfu.ca/pub/chem/>**
- b. CTI Centre for Chemistry: **<ftp://ftp.liv.ac.uk/pub/chemistry/>**
- c. Indiana University: **<ftp://fly.bio.indiana.edu/chemistry/ibmpc/>**

Some Searching Engines*Some specific searching engines:*

- a. Lycos Home Page: **<http://www.lycos.com/>**
- b. Yahoo Home Page: **<http://www.yahoo.com/>**
- c. CUI Search Engines Home Page: **<http://cuiwww.unige.ch/search-form.html>**
- d. WebCrawler Home Page: **<http://webcrawler.com>**

Pointers to a comprehensive range of searching engines:

- a. SingNet's Index: **<http://www.singnet.com.sg/public/search.html>**
- b. Internet Navigation Tools: **<http://riceinfo.rice.edu/Internet/>**
- c. Internet Search Engine: **<http://www.bbcnc.org.uW/babbage/iap.html>**