

## **Chemistry and the World Wide Web**

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### **The World Wide Web**

Any attempt at a comprehensive treatment of the impact of the World Wide Web (WWW) on the field of Chemistry is doomed to failure, so this is necessarily a brief overview (or rather a fleeting snapshot) of the "Information Superhighway" which hopes to at least focus on some of the important ways in which the WWW can be useful to chemists. Printed information about the Internet or the WWW is necessarily quickly dated<sup>1-5</sup> so that it is often better to get up to date information from the WWW itself (e.g. via one of the many WWW indexes and search engines).

The advent of the WWW has provided a new flexible medium for presenting information in a variety of formats with logical links between the information. In fact it is a natural evolution (and superset) of several pre-existing (but often still useful) approaches for accessing resources on the Internet (e.g. Email, Telnet, NNTP, FTP, Gopher).<sup>4,5</sup> Though the concept of the WWW originated in 1989,<sup>4</sup> it wasn't until the release of the first popular WWW browser, Mosaic in 1993,<sup>2</sup> that the WWW very quickly became the standard paradigm for

organising, storing and retrieving resources on the Internet. So much so that the WWW and the Internet are often thought to be synonymous.

The fundamental format type of the WWW is known as hypertext and is written in a language known as HTML (HyperText Markup Language). This format allows for text documents to be linked to other documents which may themselves be text or in fact any other document type (e.g. graphics, sound, animation, programs) which can be supported (ie. translated) by a WWW browser (e.g. Netscape Navigator, Internet Explorer) or appropriate WWW helper programs. Thus, a rich variety of information can be stored on the Internet as a network of hypertext links. Local and remote users can access such information on the WWW in a user transparent manner by means of a WWW browser. The location of resources on the Internet is specified by a standard electronic address known as a Uniform Resource Locator (URL) which has a basic structure of <protocol://host.domain/path/filename>. <sup>1-4</sup>

### **A Wealth of Chemical Resources**

There has been much hype about the growth of the Internet but based on the average of various estimates (annual growth rates ranging from 20% to 135%) it has been claimed that the Internet has been growing exponentially since 1988. This has also been reflected in the dramatic growth in the number of chemically relevant WWW sites, from a few in 1994 to over a hundred in 1995 to many thousands at present. For a specific example, there are approximately a hundred academic chemistry sites in Australia alone and about a thousand academic chemistry sites worldwide.

A summary of some useful chemical WWW links is provided below:

WWW Virtual Chemistry Library	<a href="http://www.chem.ucla.edu/chempointers.html">http://www.chem.ucla.edu/chempointers.html</a>
Australian Chemistry Network	<a href="http://apamac.ch.adfa.oz.au/OzChemNet/">http://apamac.ch.adfa.oz.au/OzChemNet/</a>
WebChemistry	<a href="http://www.latrobe.edu.au/www/webchem/">http://www.latrobe.edu.au/www/webchem/</a>
NIU Cheminformatics	<a href="http://hackberry.chem.niu.edu/">http://hackberry.chem.niu.edu/</a>
CSIR	<a href="http://www.csir.org/">http://www.csir.org/</a>
WWW Links for Chemists	<a href="http://www.liv.ac.uk/Chemistry/Links/">http://www.liv.ac.uk/Chemistry/Links/</a>
ChemWeb	<a href="http://www.chemweb.com/">http://www.chemweb.com/</a>
ChemDex	<a href="http://www.shef.ac.uk/chemistry/chemdex/">http://www.shef.ac.uk/chemistry/chemdex/</a>
WebElements	<a href="http://www.shef.ac.uk/chemistry/web-elements/">http://www.shef.ac.uk/chemistry/web-elements/</a>
ChemFinder	<a href="http://chemfinder.camsoft.com/">http://chemfinder.camsoft.com/</a>
RACI	<a href="http://www.raci.org.au/">http://www.raci.org.au/</a>
Royal Society of Chemistry	<a href="http://chemistry.rsc.org/">http://chemistry.rsc.org/</a>
ACSWeb	<a href="http://www.acs.org/">http://www.acs.org/</a>
European Chemical Society	<a href="http://ecs.tu-bs.de/">http://ecs.tu-bs.de/</a>
Royal Swedish Academy of Sciences	<a href="http://www.kva.se/">http://www.kva.se/</a>
Nobel Foundation	<a href="http://www.nobel.se/">http://www.nobel.se/</a>

One of the more useful first ports of call for finding chemical information is the WWW Virtual Library in Chemistry which contains a host of links to chemistry sites at academic institutions, and at non-profit and commercial organisations. There are also lists of chemistry resources, Chemistry Gopher and FTP Servers, and information on Chemistry and Biochemistry USENET News Groups. Good local sources of chemical information are provided by the Australian Chemistry Network at ADFA and the WebChemistry index at Latrobe, and the ChemFinder site provides a convenient way to search for chemical compounds over the WWW (see <<http://chemfinder.camsoft.com/chimia.html>> for a description).

Another example of useful chemical resources include the WWW sites for various of the national and international chemical societies e.g. our very own RACI, the Royal Society of Chemistry, the American Chemical Society (ACSWeb) and the European Chemical Society. Information can also be obtained on the Royal Swedish Academy of Sciences and the Nobel Foundation for all you budding Nobel laureates! Many of these sites allow access to resources such as press releases, conference announcements, educational resources and society journal contents listings. For example, information on the 1998 Nobel Prize in Chemistry is at <<http://www.nobel.se/announcement-98/chemistry98.html>>.

### **The Advent of Electronic Journals**

The structure of hypertext lends itself quite well to the traditional format of a scientific journal. with a typical online version composed of links to papers. The papers themselves could be composed of links to the usual main sections e.g. abstract, introduction, method, figures, tables, discussion, conclusions and references. Ideally the references themselves would be linked to the electronic versions of those papers. Of course much of this is still a pipe-dream but a few brave publishers of respectable scientific journals have taken the first few steps along the path to hypertext-based electronic journals and established WWW sites containing links to the contents pages of their paper-based journals as well as archives of supplementary information that would be too voluminous for the paper-based journal.

In some of the more computer-oriented fields, the hypertext revolution has gone all the way and some journals purely exist in the form of electronic publication of papers on and electronic access from a WWW site. Even in the somewhat conservative field of Chemistry, a number of journals have made use of the WWW. Many existing paper based journals have been made available in

online electronic editions. Some new journals have been made available only in electronic form (e.g. The Internet Journal of Chemistry), sometimes augmented by progressive volumes published on CD-ROM. The Journal of Molecular Modeling, published by Springer Electronic Media, claims to be the first fully electronic journal in Chemistry.

The most comprehensive list of chemistry journals on-line <<http://www.chemconnect.com/library/journals.shtml>> contains over 500 links to various chemistry journals. Typical examples of chemistry journals, publishers and chemical databases on the WWW follow below:

Australian Journal of Chemistry	<a href="http://www.publish.csiro.au/journals/ajc/">http://www.publish.csiro.au/journals/ajc/</a>
American Chemical Society Publications	<a href="http://pubs.acs.org/">http://pubs.acs.org/</a>
Elsevier Science	<a href="http://www.elsevier.nl/">http://www.elsevier.nl/</a>
Journal of Molecular Modelling	<a href="http://www.ccc.uni-erlangen.de/jmolmod/">http://www.ccc.uni-erlangen.de/jmolmod/</a>
Internet Journal of Chemistry	<a href="http://www.ijc.com/">http://www.ijc.com/</a>
Chemical Physics Preprint Database	<a href="http://www.chem.brown.edu/chem-ph.html">http://www.chem.brown.edu/chem-ph.html</a>
Chemical Abstracts Service	<a href="http://www.cas.org/">http://www.cas.org/</a>
STN Introduction	<a href="http://info.cas.org/stn.html">http://info.cas.org/stn.html</a>
Dialog	<a href="http://www.dialog.com/">http://www.dialog.com/</a>

A though provoking issue facing researchers, librarians and publishers of science journals is the conflict between shrinking journal acquisition budgets and the increasing price of subscriptions.<sup>7</sup> Electronic publishing is seen as a possible solution but brings with it the need to reexamine issues such as the necessity for peer review, publishing and subscription costs and the nature of information ownership.<sup>8</sup> In other fields, such as Physics, pre-prints are quite commonly distributed electronically <<http://xxx.lanl.gov>> but this is presently

uncommon in Chemistry, often because some established journals will not consider a paper for publication if preprints have been widely distributed. There has been some move to fight traditional publication restrictions by researchers and librarians beginning new independent electronic publications. Though these developments are in their infancy, it is clear that the nature of scholarly publication may undergo some changes in the future, prompted partly by ready access to electronic media such as the WWW.

### **Electronic Conferences**

One of the promising new uses of the WWW is in providing a forum for electronic conferences.<sup>9</sup> Since 1993, a significant number of chemical electronic conferences has been held with topics ranging from organic chemistry, to molecular modelling, to computational chemistry. In November 1994, the First Electronic Computational Chemistry Conference (ECCC) proved the viability of the approach (About 300 participants registered and over 60 papers were presented) and an ECCC has been held annually since with the Fifth ECCC <<http://hackberry.chem.niu.edu/ECCC5/>> due to be held during November 1998.

The WWW conferencing approach has advantages and disadvantages. Costs of attendance are minimal, assuming one has an Internet connected computer with appropriate software. Of course the feeling of really being at a conference (e.g. in Hawaii and away from the distractions of one's own institution) isn't quite there. Real conferences have the distinct advantage of one-on-one communication with scientists in close physical proximity (sometimes this may be a disadvantage!). Future online-video techniques may help address some of this, allowing for the nuances of body language in communication.

The WWW is obviously a useful means of communicating research results and ideas in a cost-effective manner but perhaps (thankfully) technology has some way to go before it can seriously compete with the advantages of physically attending a real conference.<sup>10</sup> Thus, despite the increasing popularity of electronic conferences, there is no shortage of the traditional sort of conference. Even so, hardly any respectable conference is organised without an associated WWW site for providing information and often allowing online registration. Almost paradoxically, and perhaps reflecting some of the current limitations of the WWW medium discussed above, there is no shortage of the traditional sort of conference with topics relating to the Internet/WWW and Chemistry e.g. the ChemInt'98 - Chemistry and the Internet conference <<http://www.ijc.com/ci1/>> recently held (September 1998) in California.

### **Other Uses of the WWW in Chemistry**

This article has hardly touched on many of the current and potential uses of the WWW in Chemistry. From the (academic or commercial) institutional point of view, the WWW is a cost effective method of providing information and a point of contact in a way which provides both a local, national and international outreach to other researchers, students and potential customers. Research activities and publications, useful software, on-line courses, exciting breakthroughs, annual reports, positions vacant and product descriptions are all easily handled within the WWW framework. Within a given organisation, the WWW can provide a convenient intranet capacity, in which selected information can be organised and made accessible to specific groups of users. The potential uses to which the WWW can be put in a chemical setting seem only limited by one's imagination and local computing resources.

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