

**DFN Project Chemie.DE:  
Building an Internet Information  
Service for Chemistry**

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URL for this talk:

<http://www.chemie.fu-berlin.de/chemistry/papers/iuk97/>

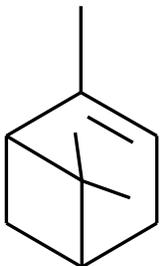
## DFN Project Chemie.DE: Purpose and Background

The WWW server to be set up shall help chemists to find **information** which is available in the Internet as well as **software** appropriate to their tasks *quickly* and *efficiently*

<http://www.chemie.de/>

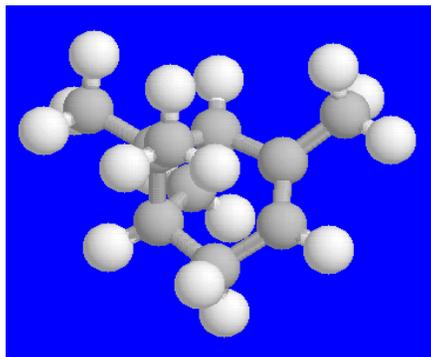
- Chemists are faced with **complex tasks**: analysis of substances, development of new products and prediction of properties, which require the application of computers to an increasing extent.
- Chemists are among the main users of **computer power**: quantum chemical calculations, molecular modeling, complicated simulations.
- The vast amount of experimental and theoretical data requires **intelligent methods of information processing**.
- Chemists can hardly cope with the **flood of information** available in the Internet and in data bases dealing with chemical or biochemical problems.
- Typical chemistry documents contain a substantial amount of **non-text information**: 2D and 3D molecular structures, spectra and mathematical formulas, which cannot be retrieved by conventional word-based search tools.
- Chemistry has a high demand of visualization calling for **multi-media presentation**: three-dimensional objects (molecules, crystals), representation of vibrations, kinetics or reaction mechanisms by means of animations or video sequences.

# Special Presentation Formats Used in Chemistry

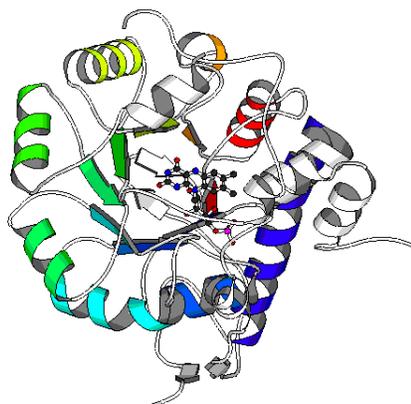


$\alpha$ -Pinene

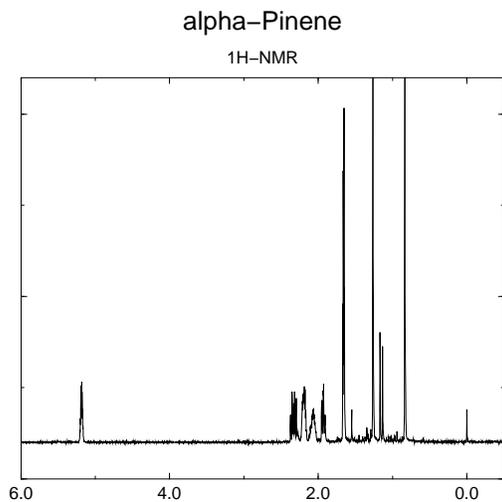
structural formulas (2D)



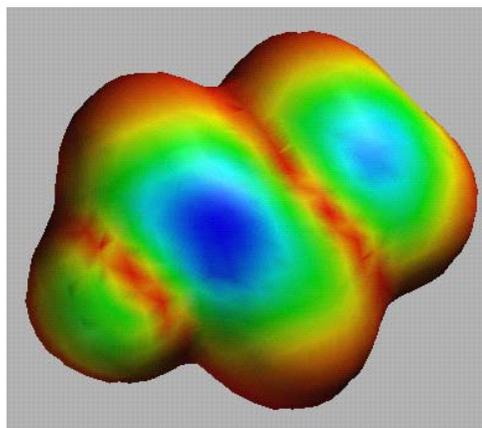
molecular models (3D)



sequences of amino acids (peptides, proteins, enzymes) or nucleotides (DNA, RNA)



spectra (NMR, IR, MS, UV, ...)



surfaces

and:

- animations
- video sequences

for visualizing:

vibrations, kinetics, reaction mechanisms

## DFN Project Chemie.DE: Aims

### Software

- **evaluation of public domain software** for chemistry and biochemistry, pointers to FTP sites or offering on local site
- data base of commercial **software products** for chemistry

### Internet Information

- list of **chemistry information servers**
- **meta index of documents** relevant to chemistry available in the Internet with convenient search methods
- compilation of **mailing lists** and **news groups** relevant to chemistry

### Dates

- calendar of German and international **conferences** and meetings

### Job Market

- list of **job** offers and applications

## DFN Project Chemie.DE: Development Tasks

- development of **search tools**, search for **molecular structures**; tools for an automated classification of documents
- compilation and offering of specialized **data bases**, e.g.: hazardous substances, thesauri for technical terms, molecular structures, occupational safety, waste disposal
- specific transport protocols, **chemical MIME** (Multipurpose Internet Mail Extensions): standardization of exchange formats
- development of **tools**, e.g. for conversions of formats, which may help in the use of software products

### Project Team:

Dr. Wolfgang Dreißig, Dr. Holger Busse (leaders);  
Hans Benedict, Thomas Richter, Claus Schröter;  
Priv.-Doz. Dr. Burkhard Kirste

### Acknowledgment:

Verein zur Förderung des Deutschen Forschungsnetzes (DFN), BMBF

## DFN Project Chemie.DE: History and Current Status

### History: our departmental WWW server

<http://www.chemie.fu-berlin.de/>

which went online in June 1993, was the very first German server in the area of chemistry. On that server, some aspects of the planned service can already be seen, such as information about hazardous substances and the beginnings of an Internet chemistry index:

<http://www.chemie.fu-berlin.de/chemistry/index/>

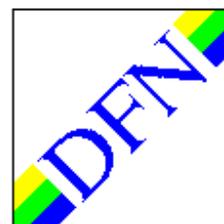
**Period of the project Chemie.DE:** 1996-11-01 – 1998-10-31

**Current status** (February 1997):

- Most of the **hardware** (PC-based) has been bought and installed.
- The **WWW server software** has been chosen and installed: **Apache**/1.1.1 with **PHP/FI** (operating system: Linux 2.0.27).
- Several **data base systems** have been considered, and **PostgreSQL** has been chosen for the construction of the software and URL data bases etc.
- **Classification systems** (attributes) for the software and chemistry document URL data bases have been discussed.
- First attempts of **gathering chemistry documents** by means of the **Harvest Broker** have been performed. The task of selecting those links to follow which are most relevant to the field of chemistry is not trivial.



Location:



## Chemie.DE

### Willkommen bei Chemie.DE Welcome to Chemie.DE

Chemie.DE ist ein vom [DFN-Verein](#) getragenes und am [Fachbereich Chemie](#) der [Freien Universität Berlin](#) lokalisiertes Projekt. Ziel des Projekts ist der

*Aufbau eines Internet-Informationssdienstes für die Chemie.*

Näheres entnehmen Sie bitte der [Projektbeschreibung](#).

Projektbeginn war der 1. 12. 1996. Im März 1997 soll der Probetrieb des WWW-Servers mit einem noch eingeschränkten Angebot aufgenommen werden.

Wenn Sie über Neuerungen auf diesem Server informiert werden wollen, hinterlassen Sie bitte hier Ihre e-mail-Adresse:




Chemie.DE is a project supported by the [DFN-Verein](#) and located at the [chemistry department](#) of the [Free University of Berlin](#). It's aim is

*building a chemistry internet information server.*

The project was started on December 1st, 1996. A limited test service will commence in March 1997.

If you want to be notified of any changes on this server, please leave your e-mail here:





# CHEMIE.DE

## Entrys in Database: links

OID	URL	Title of Page
	<input type="text"/> <input type="button" value="Query"/>	<input type="text"/> <input type="button" value="Query"/>
281526	<a href="http://crystal.biol.csufresno.edu/">http://crystal.biol.csufresno.edu/ ..</a>	CSU, Fresno Chemistry Department ..
281527	<a href="http://www.mtsu.edu/~chem/">http://www.mtsu.edu/~chem/ ..</a>	The Middle Tennessee State University De ..
281528	<a href="http://abel.mathematik.uni-stuttgart.de/">http://abel.mathematik.uni-stuttgart.de/ ..</a>	Einfuehrung in Messenger ..
281529	<a href="http://ac16.uni-paderborn.de/cic/index.h..">http://ac16.uni-paderborn.de/cic/index.h ..</a>	11. CIC-Workshop Paderborn 1996 ..
281530	<a href="http://aclinux1.chemie.uni-hamburg.de/~n..">http://aclinux1.chemie.uni-hamburg.de/~n ..</a>	MARS Online ..
281531	<a href="http://aixserv2.urz.uni-heidelberg.de:14..">http://aixserv2.urz.uni-heidelberg.de:14 ..</a>	Heidelberg Faculty of Chemistry ..
281532	<a href="http://amethyst.cbs.ogi.edu/~boswell/XOP..">http://amethyst.cbs.ogi.edu/~boswell/XOP ..</a>	EPR Simulation with Igor Pro for the Mac ..
281533	<a href="http://apamac.ch.adfa.oz.au/ozchemnet/ch..">http://apamac.ch.adfa.oz.au/ozchemnet/ch ..</a>	University College (UNSW) School of Chem ..
281534	<a href="http://ozchemnet.adfa.oz.au/OzChemNet/AS..">http://ozchemnet.adfa.oz.au/OzChemNet/AS ..</a>	The Australian Chemistry Olympiad ..
281535	<a href="http://apamac.ch.adfa.oz.au/OzChemNet..">http://apamac.ch.adfa.oz.au/OzChemNet ..</a>	Australian Chemistry Network (OzChemNet) ..
281536	<a href="http://ozchemnet.adfa.oz.au/OzChemNet/AS..">http://ozchemnet.adfa.oz.au/OzChemNet/AS ..</a>	Australia and the International Chemistr ..
281537	<a href="http://www.bruker.com/">http://www.bruker.com/ ..</a>	Bruker USA Home Page ..
281538	<a href="http://aps.org/">http://aps.org/ ..</a>	The American Physical Society ..
281539	<a href="http://www.ari.net/ars/">http://www.ari.net/ars/ ..</a>	ARSoftware Has Relocated ..
281540	<a href="http://photoscience.la.asu.edu/photosyn/">http://photoscience.la.asu.edu/photosyn/ ..</a>	Photosynthesis Center ..
281541	<a href="http://photoscience.la.asu.edu/photosyn/">http://photoscience.la.asu.edu/photosyn/ ..</a>	Nicelist ..
281542	<a href="http://magnet.chemistry.uakron.edu/MAGNE..">http://magnet.chemistry.uakron.edu/MAGNE ..</a>	MAGNET: Internet Sites ..
281543	<a href="http://www.chemheritage.org/">http://www.chemheritage.org/ ..</a>	Chemical Heritage Foundation ..
281544	<a href="http://betty-boop.unk.edu/departments/ch..">http://betty-boop.unk.edu/departments/ch ..</a>	Welcome to the Chemistry Department ..
281545	<a href="http://bilbo.edu.au/">http://bilbo.edu.au/</a>	Faculty of Chemistry, University of

<http://www.chemie.de/>

URL for this talk:

<http://www.chemie.fu-berlin.de/chemistry/papers/iuk97/>

## Concluding Remarks

- Chemists should use and make use of **electronic media**.
- Chemists should consider **online publication** of scientific results; thus, Ph. D. theses, diploma theses, talks and poster presentations could be made publicly available to a world-wide audience.
- Convenient and powerful tools for the creation of **HTML documents** or the conversion of existing documents (e.g., `rtftohtml` or `latex2html`) are available. Most sophisticated and flexible would be the use of **SGML** (Standard Generalized Markup Language); the **linuxdoc** system (offering a variety of output formats) is freely available.
- Scientific societies and groups should be encouraged to publish their **newsletters online**.
- Perhaps the installation of a central information and data service in Germany (as already available in some other countries) for the **distribution of costly scientific information** (commercial data bases and online journals) to academic sites might help universities to keep up-to-date despite decreasing budgets.