CAOS/CAMM Center – Dutch Expertise Center for Computer Assisted Chemistry

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Description

The CAOS/CAMM Center is the Dutch National Expertise center for Computer Assisted Chemistry, funded by the Dutch National Science Foundation NWO. It is an Academic Institution and it offers chemists an elaborate package of software tools, for remote use on a "central" computer system.

The emphasis is on easy accessibility, achieved by the application of menu controlled front-ends and interfaces and on integration of the various tools and data bases. An example of the latter is the interconversion of molecular structure files between structural databases, modeling software and computational chemistry programs. All available tools are presented to the user in a hierarchy of simple menus, where the tools are arranged according to their application. The Center supports its users through a combination of on-line Help facilities, practical courses and the (re)production of manuals. E-mail facilities, NEWS and Conferencing systems are used to improve the exchange of information and experience among the users, including the Center's picstaff.

All tools and programs are arranged in packages, covering four major chemical areas:

A: CAOS (Computer Assisted Organic Synthesis)
Available tools are Reaction Retrieval Systems and Fine directories and Synthesis Planning programs.

B: CAMM (Computer Assisted Molecular Modeling)
Available tools are 3-D Structural data bases and a variety of modeling programs.

C: CompChem (Computational Chemistry)
Available tools are Advanced modeling programs, visualization tools, the quantum chemistry literature database and computational tools for both Molecular Mechanics/Dynamics and Quantum Chemical calculations.

D: Area CAMMSA (Computer Assisted Macromolecular Sequence Analysis; BioInformatics)
Available tools are all major nucleic acid and protein sequence data bases and programs for data base query and retrieval, homology searching, protein analysis, nucleic acid analysis, alignment and phylogeny construction.

Expert help is available on each of the systems supported by the Center. All data bases supported by the Center are updated on a daily, weekly, monthly or quarterly basis, dependent on the rate with which new material is being produced and available. User interaction with the tools supplied is fully structure oriented whenever applicable, i.e. most input is by means of structural formulas to be drawn on the screen and output is structure oriented where appropriate.

It is the Center's policy to provide users with all documentation that is available with a program or data base, and to complement this information with on-line Help, with extra manual and "introductions" where necessary and with document files in a central document directory from which all material can be down loaded.

Network Access

Access to the Center is possible in many different ways. The route to be chosen will depend on a user's local situation. Many routes connect to the Center's terminal servers which will distribute incoming calls over the available resources.

1. DECnet. Only possible if you are setting up the connection from a local VAX in The Netherlands. Use the command SET HOST CAOS
2. TCP/IP Available if your local machine has access to Internet. (In principle world wide).

   Use the command TELNET

   caos1.caos.kun.nl(131.174.82.227) or
   caos2.caos.kun.nl(131.174.82.228)
3. X.25 In principal available world wide when you have access to an X.25 packet switching network.

   "Dial" number (0)204 18802008099 or if you are in Europe and have access to the IXI backbone (0)204 3044008699. This connection is slower than routes 1 and 2 because they use a 9.6 kb PAD. On response from the PAD answer with a <return> to connect to a terminal server which will prompt with <Local>. Type C(onnect) CAOS in response to be connected to one of the Center's nodes.

Who Can Use The Resource

Use of the Center's resources is open for all chemists employed by Dutch Chemical Research institutions, and as far as the Center's resources allow, for users outside Holland. Currently sufficient resources available.

Access is only possible at a subscription basis. Requests for a Userid and a Password should be mailed to the above e-mail address.

A subscription includes:

- a maximum of 2 simultaneous interactive processes
- free use of all CAOS/CAMM utilities for e-mail, NEWS bulletin boards, downloading, plotting, etc.
- 10 MB free disk space (additional space will cost Hfl. 500,- per 5 MB/year).
- NO additional charges (i.e. free CPU use etc.)

Current subscription rates are:

Hfl. 1500/year for each of the packages A,B and C mentioned above.
Hfl. 2250/year for package D.

A reduction is applied for combinations of packages;
Hfl. 2625/year for any two packages and Hfl. 3000 for more than 2.

For accounts opened after July 1st., the charge will be 50% of the yearly fee.

Subscriptions are automatically renewed for another year, unless the Center receives written (e-mail) notice of cancellation before November 1st.

All prices quoted above refer to Academic accounts in The Netherlands. Not-for-profit organizations pay a surcharge of 25%, as do Academic Institutions abroad. For commercial companies, individual licenses have to be negotiated on the basis of each software tool requested.

Miscellaneous

Short (1 week) trial accounts may be granted on request, at the Center's discretion. E-mail requests to the address above.

References

GOPHER access to Service description at
camms1.caos.kun.nl(131.174.82.237)