chem IT Services GbR
Leistenstrasse 44 A
D-97082 Würzburg

Tel.: 0931 7840802
Fax: 0931 7840809

info@chemits.com
www.chemits.com

Installing HyperChem for Linux

Files that will get installed:

The files that are included with the Linux distribution of HyperChem can be inspected by the following command, executed from the directory where chem.tar.tgz resides on the Linux machine:

tar -ztvf chem.tar.tgz

From this you will see that the installation consists of the seven computational modules mmplus, newton, eht, ndo, tndo, gauss, and dft that are place in the directory:

/usr/local/bin

These modules are "backend" modules that do the number crunching for HyperChem, such as molecular mechanics and quantum mechanics calculations. They are binary executables.

In addition, HyperChem needs various parameter and other important files, as it executes. These are placed in a directory:

/usr/lib/HyperChem/runfiles

Manual:

The manual consists of a chem.chm file that is place in the directory:

/usr/lib/HyperChem/HtmlHelp

This file is on-line help in the format of a Windows HtmlHelp (*.chm) file. On Linux it can be read and perused by using the utility, xchm. The xchm package can be downloaded on your Linux machine using apt-get, the Semantic Package Manager, or other Linux software for adding the additional software packages to your machine. The chem.chm file is then read into the xchm software to be perused at will. This form of manual or help file is independent of HyperChem itself and is not accessed directly from HyperChem.

Scripts:

HyperChem is capable of running scripts (HyperChem Command Language - HCL). These are placed in a *.scr file and read from the File menu. Also individual one-line script commands can be executed in a dialog box available form the menus. A directory of sample script files is included in the directory:

/usr/lib/HyperChem/scripts

Executable:

Finally, the product consists of an executable file "chem" and a set of initialization values that come from a text file "chem.ini" that is read by chem when it begins and is written by chem as it exits. The two files go together and get installed at "." or the location where the tar command that extracts the files is run. This would normally be at your home directory, such as /home/myself.

Installation:

Finally, the above files all get installed, performing an installation, by running the following command (as Super-User):

tar -zxvf chem.tar.tgz -P

If you do not know how to obtain "superuser status", contact your system administrator to execute the command for you. The principal need for superuser status is to place the backend files and runfiles in a protected global location that multiple users can access. If only you are going to use HyperChem you may still need a system administrator to extract files to these global location and then possibly move them to your local directories. The "capital P" option is required to obtain correct permissions on the installed files.

If the downloaded tgz file is in a location other than your local directory, you will need to modify the above command to name the location of the downloaded file. For example, if the file exists in the directory/etc/download, then the above command is replaced by:

tar -zxvf /etc/download/chem.tar.tgz -P

Licensing:

HyperChem for Linux is a licensed product such that the downloaded product requires a time-limited license (softlock license) to run. The product can be installed by anyone, anywhere but requires a license to run. A license allows the software to be executed on a particular machine for a specific period of time. A purchased product generally is not time-limited but runs only on one machine at a time. Site licenses allow the software to run on any machine with an appropriate IP address.

To license your evaluation copy of HyperChem for Linux, make an attempt to run the software with the command,

./chem

from the directory where it resides. A dialog box will appear that contains a 7-digit Lock Code that is a fingerprint identifying your machine. Send this 7-digit code by e-mail to:
support@chemits.com
 along with a request for a specific evaluation license. Mention the Serial Number 7339999 in your request.

We will send you back a 20-character License Code that you should type into the same dialog box mentioned above. This will allow your copy of HyperChem for Linux to run for a specified time period on that specific machine. When you exit HyperChem, the License Code will be stored in the chem.ini file and HyperChem will run as long with that license as long as the time limit on the license has not expired.

The time-limit on the license is 10 days. The license clock begins at the time the license is sent to you.