

# Setting up software for EFN115F and EFN510G

## 1 Introduction

The main software used is called ORCA and you will use a computer at the University of Iceland called Elja. ORCA is used extensively in theoretical chemistry research and has many thousand active users all over the world. Elja is a computer cluster running the Unix operating system, see <https://irhpc.github.io/is/docs/elja/bash>. ORCA is command-line based (i.e. the input and output is text) as most such software packages, and in order to use the it you need to learn how to use the Unix command line. See the document ‘A few important Unix commands’ on the course web page.

ORCA is already installed on Elja. The executable is in the directory

```
/users/home/bob9/orca_504
```

and you can use it from there, i.e. there is no need to copy it over to your home directory. It is also possible to do calculations with ORCA on your own computer. You then need to register on the ORCA forum, download an executable for the appropriate operating system (MacOS, Windows or Linux). Installation guides can be found on the ORCA website. The software is also command-line based on laptops, i.e. it does not have a graphical user interface.

In order to carry out a calculation of a molecule, the atoms in the molecule need to be specified as well as their location. The location is given by either Cartesian or internal coordinates. To create molecular coordinates and to later visualise results (molecular configuration, molecular orbitals etc.) you can install and use the Chemcraft software (it has a 150 day trial license) on your computer.

To connect to Elja, you need to use the SSH (Secure Shell) and SFTP (Secure File Transfer Protocol) protocols. Directions for installing the required software are given below.

## 1.1 Installation of ChemCraft

### On Windows computers

Installing Chemcraft on Windows is simple. Download one of the versions on the Chemcraft web site.

### On Macintosh computers

A MacOS version of Chemcraft is not available but it is possible to use the Windows version of Chemcraft via the Wine emulation environment. Here are the instructions for the installation:

1. First install the Wine software. Winebottler usually works quite well. Other options are PlayOnMac and Wineskin. If Wine complains about the lack of X11/Xquartz on your computer, you first need to install Xquartz.

- 2a. It is best to download the standalone Chemcraft program ("WinZip archive without installer") from the Chemcraft download site. Then open the Chemcraft.exe file. The Winebottler program will start and will ask whether you want to run the program or install it. Simply choose to run it. This may take some as the program is initialized on your computer.

- 2b. Another option is to download the installer ("Self-installing executable") from the Chemcraft download site and open the Installer.exe file via the Winebottler program, have Winebottler install it and create a Mac application.

**On Linux computers** Try the Linux version that is available on the Chemcraft download site. If it does not work, install the Windows version using Wine. First install a Wine program e.g. from WineHQ or it may be easier to use PlayOnLinux. Then download the Windows version of Chemcraft (either the installer or

the standalone program) and use it through Wine.

## 1.2 Connecting to Elja

Installing an SSH client:

### Windows computer

Unlike MacOS and Linux, the Windows operating system is not built on Unix and does not have a command-line Unix interface that can be used to connect to a computer running Unix, such as Elja. It is therefore necessary to set up an SSH client to connect to Elja. There are many clients available. It is recommended to install **MobaXterm** (<https://mobaxterm.mobatek.net/>).

1. Download the MobaXterm SSH client from its web site:
2. Install the program.
3. Open the program.
4. Then click on "sessions" and select SSH. Find the tab "Basic SSH settings" and type the following into the "Remote host" box: elja.hi.is. Next time you start the program, mobaXterm will know the address for Elja.

Furthermore, in order to use X11 forwarding, you need to set up a small program called "Xming" (<https://sourceforge.net/projects/xming/>)

### Macintosh and Linux computers

MacOSX and Linux are a Unix based operating systems and they come with a command-line interface. On Macs, go to the Utilities directory under Applications, and find the Terminal application. Linux also has a built-in shell that you can use right away. To connect to Elja, type the following SSH command

```
ssh -X username@elja.hi.is
```

## 1.3 Once you are connected to Elja

Once connected you should be greeted by a welcome message. Through this window you can type in Unix commands such as change directory (cd), list files (ls),

create a directory (mkdir) or even submit an ORCA calculation. Various useful Unix commands are summarized in the document 'A few important Unix commands' on the course web site. To disconnect from Elja, you can either type the exit command or simply close the window.

**Advanced MacOS/Linux tip:** It is also possible to set up an alias for the SSH command in your MacOS or Linux computer shell in order to reduce effort. Add the line `alias sol='ssh -X username@elja.hi.is` in your `.bash_profile` on your Mac/Linux computer.

Furthermore, to avoid typing in the password each time, you can set up SSH keys.

## 1.4 Copying files between your computer and Elja

### Windows:

The mobaXterm program is both an SSH shell client and an SFTP program so you do not need to set up another program for copying files.

### MacOS:

It is convenient to have a program with a graphical interface to exchange files between your Mac and Elja. Filezilla is a free FTP & SFTP client that works well. Other options are Captain FTP, Transmit. When downloading Filezilla, avoid the installer as it contains adware.

Installing Filezilla on MacOS for use with Elja as follows:

1. Download the installer from <https://filezilla-project.org/download.php?type=client>.
2. Launch the installer. Ignore everything (close windows) concerning Zipcloud that you do not need.
3. Open the program.
4. Open the Site Manager. File -> Site Manager (Command+S). Add a New Site and change the name from "New Site" to "Elja". In the "Host:" field type `elja.hi.is`, in "Port:" add 1047. Change Protocol from FTP to SFTP. Change "Lo-

gon Type:" from Anonymous to Normal and then fill in your username and link your private key that you have been given to Elja.

5. Connect to the Server by clicking Connect. Say yes to trusting the Host if asked. You should now be connected to Elja.

6. You can now easily drag and drop files between your computer (left side) and Elja (the remote computer) on the right.

Note that it is always best to go to the Site Manager to connect File -> Site Manager (Command+S) and double-click the Elja entry you previously created. Typing in the hostname in the main window when you want to connect to Elja, will not work, unless you add "sftp://elja.hi.is" in the "Host:" field.