

# Schrödinger Product Installation on Linux

The instructions below are for a new installation of Schrödinger software on a typical Linux platform. If you need more details or encounter problems, refer to the [Installation Guide](#), which is included at the top level of the DVD or the download along with these instructions.

## Checking your system

1. Check that your system has sufficient disk space:

```
df -h
```

To install all products, 6 GB is needed. 11 GB is needed for the PDB, and 10 GB for other Prime third-party databases.

2. Check that you are installing on a supported operating system.

See [Section 2.1.3](#) and [Section 2.1.4](#) of the *Installation Guide* for a list.

## Installing the software

3. If installing from DVD, mount the product DVD.

You must have a DVD-ROM drive or a DVD-R Read/Write or DVD+/-R Read/Write drive. DVD+R Read/Write drives cannot read our DVDs.

If installing from a download, extract the tar file:

```
tar -xvf Schrodinger_Internet_Download.tar
```

4. Change to the top-level directory on the DVD or the download:

```
cd topleveldir
```

For a download this directory should be the subdirectory `Schrodinger_Internet_Download` in the directory you extracted the tar file.

5. Run the install script:

```
sh ./INSTALL
```

Using `sh` is sometimes necessary when installing from DVD.

6. Enter the information requested by the `INSTALL` script.

This includes the installation directory (which is created if necessary) and a scratch directory. See [Section 3.3](#) of the *Installation Guide* for details.

**You cannot install a new Schrödinger Suite into the same directory as a previous Suite!**

7. Set the `SCHRODINGER` environment variable to the installation directory:

```
bash:      export SCHRODINGER=installdir
```

```
csh/tcsh: setenv SCHRODINGER installdir
```

8. Set the `SCHRODINGER_PYTHONPATH` environment variable if `PYTHONPATH` is defined:

```
bash:      export SCHRODINGER_PYTHONPATH=" "
```

```
csh/tcsh: setenv SCHRODINGER_PYTHONPATH
```

### Setting up access to remote hosts

9. Add entries to `$(SCHRODINGER)/schrodinger.hosts` for all hosts or batch queues on which the software will be run. Do not remove the `localhost` entry.

See [Section 6.1](#) and [Section 6.3](#) of the *Installation Guide* for details. The minimum required for a host entry is  
name: *hostname*

10. Set up passwordless `ssh` access to all hosts on which the software will be run.

See [Section 6.2](#) of the *Installation Guide* for details.

11. Configure any clusters if necessary (see [Section 6.5](#) of the *Installation Guide*).

### Setting up licensing

12. Log on to the license server host (if you are not already logged on to it).

13. Run `machid` to obtain information for the license:

```
$(SCHRODINGER)/machid > machid.out
```

14. Send the output of `machid` to `help@schrodinger.com` to obtain a license.

15. When you receive the license information, which is sent as an attachment, save it as `$(SCHRODINGER)/license`. You can overwrite the existing file, which is a placeholder.

16. On the license server host, start the license server, and check that it is running.

```
licadmin SERVERUP  
licadmin STAT
```

See [Chapter 5](#) of the *Installation Guide* for details.

### Checking the installation

17. Check that the driver for your graphics card is up to date.

18. Run the installation checker (see [Section 6.6](#) of the *Installation Guide*):

```
$(SCHRODINGER)/installation_check
```

19. Start Maestro to ensure that it is correctly installed.

```
$(SCHRODINGER)/maestro &
```

20. Choose **Manuals Index** from the **Help** menu to ensure that the PDF viewer is working correctly from Maestro.

21. Choose **Online Help** from the **Help** menu to ensure that the browser is working correctly from Maestro.