



# Gaussian 16 Installation Instructions for Mac OS X

In order to run Gaussian 16, several UNIX environment variables must be set in each user's account. If you are comfortable using UNIX, Gaussian 16 can be set up using the [normal instructions for binary UNIX systems](#). The following alternate instructions make minimal use of UNIX commands. These instructions are appropriate for both the full program and for the Gaussian 16 Utilities.

## 1. Install the program

Insert the Gaussian 16M DVD. Open the **tar** folder, and double-click the **M\*.tbz** file; the name will vary somewhat with different revisions and depending on whether you are installing the full program or just the utilities. On most systems, Archive Utility will be started and the **.tbz** file will be expanded to a folder named **g16** on either your **Desktop** or in your **Downloads** folder (if the latter exists).

After Archive Utility has finished expanding the file, drag the resulting **g16** folder to the desired location for the G16 binaries (or the G16 Utilities). The usual installation location is the **Applications** folder. Do *not* rename the **g16** folder. There is no need to modify any files inside the **g16** folder in order to install the G16 binaries or the utilities. Note that the full directory path to the **g16** folder cannot contain any spaces.

## 2. Determine your default UNIX shell

User accounts originally created using Mac OS X 10.0.x, 10.1.x, or 10.2.x default to using the **tcsh** shell. Accounts created using Mac OS X 10.3.x or later default to the **bash** shell. To determine which shell your account uses, open a Terminal window and type the following command:

```
$ echo $SHELL
```

Notes:

- The initial **\$** above is the shell prompt and should not be typed. Your prompt may look different.
- The Terminal application is found in the **Applications/Utilities** folder.

Follow the instructions in the next step for the shell you are using.

## 3. Set the UNIX environment variables

Each user who will run Gaussian must perform this step. Mac OS X prevents the user from viewing or editing certain UNIX files from the Finder, but one can run a few simple UNIX commands to get around this limitation for specific files. Open a Terminal window. Run the following commands:

```
tcsh shell  
$ cd  
$ touch .login  
$ ln -s .login my_login
```

```
bash shell  
$ cd  
$ touch .bash_profile  
$ ln -s .bash_profile my_profile
```

Exit the Terminal program and open the file **my\_login** or **my\_profile** with a text editor such as TextEdit. Assuming that the **g16** folder was placed in the **Applications** folder, add the two lines for your shell to the file (the file may be empty at this point; if not, add these lines to the end of the file):

```
tcsh shell  
setenv g16root /Applications  
source $g16root/g16/bsd/g16.login
```

```
bash shell  
export g16root=/Applications  
. $g16root/g16/bsd/g16.profile
```

You may also want to add a third line to define a destination directory for G16M temporary files. For example:

```
tosh shell  
setenv GAUSS_SCRDIR /dir
```

```
bash shell  
export GAUSS_SCRDIR=/dir
```

where *dir* is the full path to the selected scratch folder: e.g., **/Users/your\_username/Scratch**. You will need to create the specified folder if it does not already exist.

Note that if you already have lines in the **.login** or **.profile** file which refer to g09, g03 or some earlier version, you should replace them with the above lines. Save the file as plain text (not RTF) and exit. You are now ready to install GaussViewM, following the steps on its instruction sheet.

### **Additional Setup Step when Multiple Users will run G16M**

If multiple users will log into the Macintosh computer and run G16M, then they must all be placed into the same group, and that group must be the owner of the G16M software files. The latter can be accomplished with the **chgrp -R** command. For example, the following command will set the group ownership of the G16M files to group *chem* (assuming the same installation location as above):

```
$ sudo chgrp -R chem /Applications/g16
```

These steps are essential on systems where users are placed into separate, individual groups by default. You may need to ask your system administrator to help you set up things properly.