



Molecular
Simulations

Molecular Simulations
INSTALLATION
GUIDE

Version 3.0

February 17, 1992

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Chapter 1

Installation on Titan Workstations

This chapter describes how to install Molecular Simulations software products (BIOGRAF, POLYGRAF, NMRgraf, and Polaris) on a Titan workstation. If the system has been configured correctly, this installation should take less than an hour. No compilations are performed, as all images are distributed in final linked form. The installation consists of creating an msi user account, loading the tape into a local directory tree, and configuring each user account to invoke the setup script during shell creation. Super user privilege is only needed to set up the software account. No changes are made to the operating system.

Caution: Please review all of the instructions before you start and follow them exactly. Failure to perform a step, or changes to the installation procedure will probably prevent the program from functioning correctly. Please contact MSI Customer Technical Support at (617) 487-7875 if you have any questions about the installation.

1.1 Hardware and System Configuration

All Titan workstations are supported by MSI software, including the 1500 (P2 processor) and the 750 and 3000 models (P3 processors). G2 and G3 graphics are supported for Doré graphics on the Titan workstation monitor. Required and recommended hardware options are described below:

Required Titan Hardware
Titan workstation
32 MB main memory
380 MB disk
Extended graphics option

Recommended Titan Hardware
Second 380 MB disk Dial box

Since MSI programs contain so many functions, they are very large and require a large swap partition in order to run. Approximately 90 MB of swap space is required, but MSI recommends that 175 MB of swap area be allocated to comfortably accommodate the MSI software and the necessary windows.

Recommended Titan Swap Space
175 MB

The amount of swap area available may be obtained by using the `nvr` and `dvhtool` commands. `Dvhtool` must be performed as root. First find out which is the swap partition. Type:

```
nvr
```

Look at the line labeled `swapdev`, typically:

```
swapdev=scsi(1,5,2)
```

The swap partition number is the last number of `swapdev` (normally 1, but 2 in our example for clarity). Using this fact, you run `dvhtool` to get the partition size:

```
dvhtool
```

Warning: `dvhtool` has the power to really foul up your disk system. It can even destroy a volume, so do not deviate from the following instructions.

Type read at the command prompt:

```
Command? (read, vd, pt, dp, write, bootfile, or quit): read
```

Use first two numbers of `swapdev` to construct the volume header name from the pattern `/dev/dsk/cxxyvh`, substituting for `x` and `y`. For our example above, the first two numbers are 1 and 5, yielding the name `/dev/dsk/c1d5vh`. Enter this name at the volume prompt:

```
Volume? /dev/dsk/c1d5vh
```

Finally type the `pt` command to get the partition sizes:

```
Command? (read, vd, pt, dp, write, bootfile, or quit): pt
```

Look at the first column, labeled "part" (for partition number). Examine the entry for the swap partition number (the last number of the swapdev entry, 2 in our example):

part	n_blks	1st_blk	type	size
0:	82080	1080	sysv	80 MB
1:	66150	83160	sysv	64 MB
2:	179820	149310	sysv	175 MB
etc.				

The swap partition size is the number in the "size" column, 175 MB in our example. Now type ^c to terminate dvhtool. That is, hold down the key labeled 'control' and type the letter c.

MSI strongly recommends that the largest possible swap partition be configured, preferably at least 175 MB. If necessary, consult your documentation on how to reconfigure your system.

The following software must be installed before MSI software installation is begun:

Required Titan 1500 Software (P2 Processor)
Titan 2.2

Required Titan 750 & 3000 Software (P3 G2)
Titan 3.01 Rev A

Required Titan 3000 Software (P3 G3)
Titan 4.0 Pat1

Please contact MSI Customer Service before attempting to deviate from these specifications.

Optional Titan 1500 Software (P2 Processor)
Titan FORTRAN 2.2
Titan NFS

Optional Titan 750 & 3000 Software (P3 G2)
Titan FORTRAN 3.0.1 Beta2
Titan NFS

Optional Titan 750 & 3000 Software (P3 G3)
Titan FORTRAN 3.0.1 Beta2
Titan NFS

Note that FORTRAN is needed only for those users who relink MSI programs with FORTRAN user routines, and NFS is needed for most systems operating on a network.

1.2 Software Installation

There are three basic operations that must be performed in order to install this Molecular Simulations software: 1) creation of the msi account, 2) reading the magnetic tape, and 3) modification of the *.cshrc* file. If you are starting from scratch, all of the steps must be performed. If you have an appropriate user account, you may skip the first section.

It is recommended that a separate account be created that will have ownership of the MSI software files but that will allow other users to run the program as well. You may choose not to create an msi account, but in that case you must perform an alternative to step 8. To setup the account, ask your system manager, consult the manual that came with the computer, or use the procedure outlined below. All of the steps in the first section must be performed by the super user (root).

The instructions throughout this manual assume that the MSI software will be owned by a user named msi. In this example, the user id is 345, and the group id is 345. *You must use id numbers that will not conflict with other accounts on your system.* The files will be loaded into the msi home directory on the *usr* partition. *You should modify the pathnames in the instructions to reflect your particular situation.*

1.3 Creating the MSI User Account

- 1) Log onto the computer as root.
- 2) Use the `df` command to determine which of your disk partitions has sufficient space to load the MSI software. It requires approximately 30 MB of disk space. `Df -b` reports sizes in kilobyte blocks; so look for approximately 30,000 blocks "available". Type the command:

```
df -b
```

- 3) Identify a partition with at least 30,000 blocks available and create the user account by editing the */etc/passwd* file. Add the following line, substituting your correct pathname:

```
msi::345:345:MSI Software:/usr/msi:/bin/csh
```

- 4) Next create the home directory for this account and set the ownership and access rights with the commands below.

```
cd /usr
mkdir msi
chown msi msi
chgrp 345 msi
chmod 755 msi
```

This gives msi permission to read, write, or execute files in the home directory. Other users will be able to read or execute these files but not change or delete them. It is recommended that a password be set for this account. To do so, simply follow the prompts after typing:

```
passwd msi
```

1.4 Loading the Files from Tape

- 5) Log off of the computer as root.
- 6) Log on as msi. The rest of the steps should not be performed as root or you may have permissions problems. If you make the mistake and tar the tape as root, it is best to remove the files and start over as msi.
- 7) The standard distribution medium for Titan workstations is a 1/4 inch high-density cartridge tape. Mount the tape in the tape drive and type:

```
cd      (to make sure that you are in the msi home directory)
tar xvf /dev/rmt/c0d6h
```

Tar will report each file copied from the tape to the disk.

1.5 Installation of Shell Scripts

Each of the steps in this section must be performed once by each user who wishes to run the program.

- 8) Perform this step if you have loaded the software into an msi account. After logging into the user account, type the following command:

```
cat ~msi/biogv300/.setup300>>~/cshrc
```

This command adds two commands to your *.cshrc* file. One defines a pointer to the software directory. The other executes a shell script which defines some useful aliases and sets the environmental variables necessary to run the program.

- 8a) Alternatively, if you have chosen not to install the software in an msi account, you will need to edit your *.cshrc* file to include the lines shown below:

```
setenv MSIUSR /usr/your_directory_pathname
source $MSIUSR/biogv300/.setmsi300
```

substituting for "*/usr/your_directory_pathname*" the complete pathname of the directory in which you have installed the MSI software files.

- 9) If you have an earlier version of this MSI software, it is necessary to remove all old `setenv` and `alias` commands from your `.cshrc` file. In particular, please remove the command, `setenv BIOVER <version number>`, and any references to `BIOVER`. Also remove the command, `source /biograf/biogv${BIOVER}/bg_login.csh`, from your `.login` file.

Note: If you have setup a completely new user account from which you will run the MSI software, you may need to establish a variety of default settings for your account. At the very least, you should make sure that `/usr/X11/bin` is in your path. If it is not, include the following line in your `.cshrc` file:

```
set path=($path /usr/X11/bin)
```

For computers with G2 graphics, you may also want to create a file, `.xdesktop`, in your home directory to create a suitable window from which you can run the program. It should contain the line:

```
xterm -geometry 80x64+10+90&
```

For computers with G3 graphics, instead of the `.xdesktop` file, you should use a file, `.xsession`, in your home directory, containing the lines:

```
mwm&
xterm -geometry 80x47+10+120 -T `hostname` &
exec xterm -geometry 80x5+10+0 -n console -T console
```

- 10) Log out and then log in again so as to execute the new commands that you just entered into your `.cshrc` file. If there are command lines in your `.cshrc` file that the system doesn't understand, it will not finish the script and the aliases may not be defined.
- 11) Run the COMSTRUCT procedure by typing:

```
comstruct
```

COMSTRUCT allows you to configure the system to run the program in whatever way you choose. Select the program that you wish to run when asked to do so. Initially, it is easiest to hit only a carriage return in response to the questions in COMSTRUCT, selecting the default values. Later, when you better understand your preferred environment, you may customize your setup. Refer to the COMSTRUCT User's Guide, Appendix A in this document, for help as necessary.

You may use an alias of your own if you wish instead of the suggested default. However, if you use another alias or have COMSTRUCT place files in any directory other than your home directory, you will need to include an alias command in your `.cshrc` file so that the system recognizes your particular alias. Running COMSTRUCT generates a `.doc` file, the name of which is the alias you chose with `.doc` appended to it. The `.doc` file contains an

alias command to include in the `.cshrc` file for non-default aliases or when using another default directory. If you change `.cshrc`, log out and back in again.

Note: The Titan allows file names of only 14 characters in length. If a longer name is used, it will be truncated. As long as the resulting name is unique, no problem will result.

1.6 Running the Software

You should now be ready to run the MSI software. Before doing so, make sure that you have Xwindows running. If not, start it at this time by typing:

```
xstart
```

From the resulting window, you may run the desired MSI program by typing the alias you selected when you ran COMSTRUCT, *e.g.*:

```
biograf
```

To create additional configurations, run COMSTRUCT again as desired, selecting the necessary options to run the program in the way you choose. In order to execute the program in these new configurations using custom aliases, you must edit your `.cshrc` file to include the alias commands shown in the `.doc` files generated by COMSTRUCT. You may then safely delete the `.doc` files.

If upon starting the program, you receive an error message stating that there has been an authorization failure, please note the message and report it to MSI customer support. In most cases, such a message indicates that your software tape was made before your system id was known, resulting in an invalid authorization code.

You may obtain your system id by typing:

```
getsn
```

Report the output from `getsn` to MSI customer support, and they will send you the necessary changes that must be made to your authorization file. To make those changes, edit the file:

```
$MSIUSR/biogv300/exe/auth300.fil
```

1.7 Enabling the Stereo Monitor

A stereo monitor may be purchased for the Titan which allows the user to view images in three dimensions. In order to enable the stereo monitor, however, you must first set up an alias command which will execute the stereo version of the program. This is described in steps 1 through 4 and must be performed only once. Steps 5 through 11 must be done *after every log in* if stereo mode is desired.

Setting up the Alias Command (done only once)

1. Run COMSTRUCT using the alias command you wish to use to execute the stereo version. *e.g.*, `biostereo` or `polystereo`.
2. Edit the resulting `.def` file to include the line:

```
L_STEREO YES
```

3. Include a line in your `.cshrc` file defining the new alias similar to those used for your other aliases.
4. Log out and back in again.

Getting into Stereo Mode (done after every log in)

5. Enter the Xwindows environment by typing:

```
xstart -stereo
```

6. Type:

```
xterm -display unix:0.1&
```

7. Hold down ALT and press the F2 key as a toggle to go into the stereo screen environment.

8. Type:

```
setenv DISPLAY unix:0.1  
awm&
```

9. Run the program in stereo mode by typing the alias command set up previously, *e.g.*:

```
biostereo
```

10. Use the F5 key to activate the stereo mode (F5 toggles you back and forth between stereo and normal modes).
11. It may be necessary to reposition the window using **Move Opaque** in the WindowOps menu.

Installation of the MSI software is now complete.

Chapter 2

Installation on Silicon Graphics Workstations

This chapter describes how to install Molecular Simulations software products (BIOGRAF, POLYGRAF, NMRgraf, and Polaris) on a Silicon Graphics workstation. If the system has been configured correctly, this installation should take less than an hour. No compilations are performed, as all images are distributed in final linked form. The installation consists of creating an msi user account, loading the tape into a local directory tree, and configuring each user account to invoke the setup script during shell creation. Super user privilege is only needed to set up the software account. No changes are made to the operating system.

Caution: Please review all of the instructions before you start and follow them exactly. Failure to perform a step, or changes to the installation procedure will probably prevent the program from functioning correctly. Please contact MSI Customer Technical Support at (617) 487-7875 if you have any questions about the installation.

2.1 Hardware and System Configuration

IRIS and INDIGO workstations are supported by MSI software. This includes the Personal IRIS and the Power IRIS models. GL graphics is supported on the workstation monitors. Required and recommend hardware options are described below.

Required Silicon Graphics Hardware
SGI workstation 16 MB main memory 380 MB disk Super level graphics (G, TG, GTX)

Recommended Silicon Graphics Hardware
Second 380 or larger MB disk Dial box

Note: Using the operating system, 4D1-3.3.2 or greater with the default swap space, MSI has not experienced any problems due to swap limitations. However, it is possible that if you model very large molecules, run several copies of the program at one time, or use many program functions all at one time, you could exceed the available space. If that happens, please contact MSI Customer Support for help in reconfiguring your swap space.

The following software must be installed before MSI software installation is begun:

Required Silicon Graphics Systems Software
4D1-3.3.2 or greater Xwindows

Please contact MSI Customer Service before attempting to deviate from these specifications.

Optional Silicon Graphics Systems Software
FORTRAN Option Development System NFS Option

Note that FORTRAN is needed only for those users who relink MSI programs with FORTRAN user routines, and NFS is needed for most systems operating on a network.

2.2 Software Installation

There are three basic operations that must be performed in order to install this Molecular Simulations software: 1) creation of the msi account, 2) reading the magnetic tape, and 3) modification of the `.cshrc` file. If you are starting from scratch, all of the steps must be performed. If you have an appropriate user account, you may skip the first section.

It is recommended that a separate account be created that will have ownership of the MSI software files but that will allow other users to run the program as well. You may choose not to create an

msi account, but in that case you must perform an alternative to step 8. To setup the account, ask your system manager, consult the manual that came with the computer, or use the procedure outlined below. All of the steps in the first section must be performed by the super user (root).

The instructions throughout this manual assume that the MSI software will be owned by a user named msi. In this example, the user id is 345, and the group id is 345. *You must use id numbers that will not conflict with other accounts on your system.* The files will be loaded into the msi home directory on the *usr* partition. *You should modify the pathnames in the instructions to reflect your particular situation.*

2.3 Creating the MSI User Account

- 1) Log onto the computer as root.
- 2) Use the `df` command to determine which of your disk partitions has sufficient space to load the MSI software. It requires approximately 30 MB of disk space. `Df -k` reports sizes in kilobyte blocks; so look for approximately 30,000 blocks "available". Type the command:

```
df -k
```

- 3) Identify a partition with at least 30,000 blocks available and create the user account by editing the `/etc/passwd` file. Add the following line, substituting your correct pathname:

```
msi::345:345:MSI Software:/usr/msi:/bin/csh
```

- 4) Next create the home directory for this account and set the ownership and access rights with the commands below.

```
cd /usr
mkdir msi
chown msi msi
chgrp 345 msi
chmod 755 msi
```

This gives msi permission to read, write, or execute files in the home directory. Other users will be able to read or execute these files but not change or delete them. It is recommended that a password be set for this account. To do so, simply follow the prompts after typing:

```
passwd msi
```

2.4 Loading the Files from Tape

- 5) **Log off of the computer as root.**
- 6) Log on as `msi`. The rest of the steps should not be performed as root or you may have permissions problems. If you make the mistake and tar the tape as root, it is best to remove the files and start over as `msi`.
- 7) The standard distribution medium for Silicon Graphics workstations is a 1/4 inch high-density cartridge tape. If you have only a low-density tape drive, you will need a low-density software tape. Mount the tape in the tape drive and type:

```
cd          (to make sure that you are in the msi home directory)
tar xvo
```

Tar will report each file copied from the tape to the disk.

2.5 Installation of Shell Scripts

Each of the steps in this section must be performed once by each user who wishes to run the program.

- 8) Perform this step if you have loaded the software into an `msi` account. After logging into the user account, type the following command:

```
cat ~msi/biogv300/.setup300>>~/ .cshrc
```

This command adds two commands to your `.cshrc` file. One defines a pointer to the software directory. The other executes a shell script which defines some useful aliases and sets the environmental variables necessary to run the program.

- 8a) Alternatively, if you have chosen not to install the software in an `msi` account, you will need to edit your `.cshrc` file to include the lines shown below:

```
setenv MSIUSR /usr/your_directory_pathname
source $MSIUSR/biogv300/.setmsi300
```

substituting for "`/usr/your_directory_pathname`" the complete pathname of the directory in which you have installed the MSI software files.

- 9) If you have an earlier version of this MSI software, it is necessary to remove all old `setenv` and `alias` commands from your `.cshrc` file. In particular, please remove the command, `setenv BIOVER <version number>`, and any references to `BIOVER`. Also remove the command, `source /biograf/biogv${BIOVER}/bg_login.csh`, from your `.login` file.

- 10) Log out and then log in again so as to execute the new commands that you just entered into your `.cshrc` file. If there are command lines in your `.cshrc` file that the system doesn't understand, it will not finish the script and the aliases may not be defined.
- 11) Run the COMSTRUCT procedure by typing:

```
comstruct
```

COMSTRUCT allows you to configure the system to run the program in whatever way you choose. Select the program that you wish to run when asked to do so. Initially, it is easiest to hit only a carriage return in response to the questions in COMSTRUCT, selecting the default values. Later, when you better understand your preferred environment, you may customize your setup. Refer to the COMSTRUCT User's Guide, Appendix A in this document, for help as necessary.

You may use an alias of your own if you wish instead of the suggested default. However, if you use another alias or have COMSTRUCT place files in any directory other than your home directory, you will need to include an alias command in your `.cshrc` file so that the system recognizes your particular alias. Running COMSTRUCT generates a `.doc` file, the name of which is the alias you chose with `.doc` appended to it. The `.doc` file contains an alias command to include in the `.cshrc` file for non-default aliases or when using another default directory. If you change `.cshrc`, log out and back in again.

2.6 Running the Software

You should now be ready to run the MSI software. Before doing so, make sure that you have Xwindows running. If not, start it at this time by typing:

```
Xsgi&
```

It will not be necessary to start Xwindows manually if you are running OS 4.0 or greater. Now run the desired MSI program by typing the alias you selected when you ran COMSTRUCT, *e.g.*:

```
biograf
```

To create additional configurations, run COMSTRUCT again as desired, selecting the necessary options to run the program in the way you choose. In order to execute the program in these new configurations using custom aliases, you must edit your `.cshrc` file to include the alias commands shown in the `.doc` files generated by COMSTRUCT. You may then safely delete the `.doc` files.

If your system has the new model dial box (the one without the companion button box), then you should insert the following line at the end of your `.login` file:

```
./usr/sbin/dialwarp 0 5
```

This command configures the operation of the new dial box to correspond closely to the old dial box, multiplying the number of ticks sent by five.

If upon starting the program, you receive an error message stating that there has been an authorization failure, please note the message and report it to MSI customer support. In most cases, such a message indicates that your software tape was made before your system id was known, resulting in an invalid authorization code.

You may obtain your system id by typing:

```
get sn
```

Report the output from `get sn` to MSI customer support, and they will send you the necessary changes that must be made to your authorization file. To make those changes, edit the file:

```
$MSIUSR/biogv300/exe/auth300.fil
```

2.7 Enabling the Stereo Monitor

A stereo monitor may be purchased for the Iris which allows the user to view images in three dimensions. In order to enable the stereo monitor, you must perform the following steps.

1. Turn on the switch on the stereo monitor.
2. Turn on your stereo glasses.
3. Use the F4 key to activate the stereo mode.

Installation of the MSI program is now complete.

Chapter 3

Installation on IBM RISC System/6000 Workstations

This chapter describes how to install Molecular Simulations software products (BIOGRAF, POLYGRAF, NMRgraf, and Polaris) on an IBM RISC System/6000 (RS6000) workstation. If the system has been configured correctly, this installation should take less than an hour. No compilations are performed, as all images are distributed in final linked form. The installation consists of creating an msi user account, loading the tape into a local directory tree, and configuring each user account to invoke the setup script during shell creation. Super user privilege is only needed to set up the software account. No changes are made to the operating system.

Caution: Please review all of the instructions before you start and follow them exactly. Failure to perform a step, or changes to the installation procedure will probably prevent the program from functioning correctly. Please contact MSI Customer Technical Support at (617) 487-7875 if you have any questions about the installation.

3.1 Hardware and System Configuration

All RS6000 workstations except the model 730 and those using GTO graphics are currently supported by MSI software. Required and recommended hardware options are described below.

Required RS6000 Hardware
RS6000 workstation
16 MB main memory
400 MB disk
24 Bit 3-D color graphics processor

Recommended RS6000 Hardware
800 MB disk 16 MB main memory

Since MSI programs contain so many functions, they are very large and require a large swap partition in order to run. Approximately 90 MB of swap space is required, but MSI recommends that 150 MB of swap area be allocated to comfortably accommodate the MSI software and the necessary windows.

Recommended RS6000 Swap Space
150 MB

The amount of swap area available may be obtained by using the `lspcs` command:

```
% lspcs -a
```

Note the quantities in the "size" column. The sum of these is the largest available swap area (expressed in MB).

If you used the default configuration values when your system software was installed, there may not be sufficient swap area available to run your MSI program. If necessary, consult the IBM documentation on how to reconfigure your system (the `smitt` utility allows the swap space to be increased easily).

Note: The recent versions of AIX have a file, `/etc/security/limits`, which contains several limits. Unless you modify that file, you will not be able to allocate sufficient swap space for the program to run. We recommend that you comment out all of the limits in the section of this file labeled "defaults". You must be root to do so.

The following software must be installed before MSI software installation is begun:

Required RS6000 Systems Software
AIX 3.1.5 or 3.1.6 FORTRAN Runtime Environment 2.1.7

Please contact MSI Customer Service before attempting to deviate from these specifications.

Optional RS6000 Systems Software
FORTRAN Compiler NFS

Note that FORTRAN is needed only for those users who relink MSI programs with FORTRAN user routines, and NFS is needed for most systems operating on a network.

3.2 Software Installation

There are three basic operations that must be performed in order to install this Molecular Simulations software: 1) creation of the msi account, 2) reading the magnetic tape, and 3) modification of the `.cshrc` file. If you are starting from scratch, all of the steps must be performed. If you have an appropriate user account, you may skip the first section.

It is recommended that a separate account be created that will have ownership of the MSI software files but that will allow other users to run the program as well. You may choose not to create an msi account, but in that case you must perform an alternative to step 8. To setup the account, ask your system manager, consult the manual that came with the computer, or use the procedure outlined below. All of the steps in the first section must be performed by the super user (root).

The instructions throughout this manual assume that the MSI software will be owned by a user named msi. In this example, the user id is 345, and the group id is 345. *You must use id numbers that will not conflict with other accounts on your system.* The files will be loaded into the msi home directory on the `usr` partition. *You should modify the pathnames in the instructions to reflect your particular situation.*

3.3 Creating the MSI User Account

- 1) Log onto the computer as root.
- 2) Use the `df` command to determine which of your disk partitions has sufficient space to load the MSI software. It requires approximately 25 MB of disk space. `Df` reports sizes in kilobyte blocks; so look for approximately 25,000 blocks "available". Type the command:

```
df
```

- 3) Use the `smit` utility to create an msi user account. If the `usr` partition has sufficient space, use `/usr/msi.` as the home directory.
- 4) Next create the home directory for this account and set the ownership and access rights with the commands below.

```
cd /usr
mkdir msi
chown msi msi
chmod 755 msi
```

This gives msi permission to read, write, or execute files in the home directory. Other users will be able to read or execute these files but not change or delete them. It is recommended that a password be set for this account. Use `smit` to do so.

3.4 Loading the Files from Tape

- 5) **Log off of the computer as root.**
- 6) Log on as `msi`. The rest of the steps should not be performed as root or you may have permissions problems. If you make the mistake and tar the tape as root, it is best to remove the files and start over as `msi`.
- 7) The standard distribution medium for RS6000 workstations is a 1/4 inch high-density cartridge tape. Mount the tape in the tape drive and type:

```
cd          (to make sure that you are in the msi home directory)
tar xvBf /dev/rmt0.4
```

Tar will report each file copied from the tape to the disk.

3.5 Installation of Shell Scripts

Each of the steps in this section must be performed once by each user who wishes to run the program.

- 8) Perform this step if you have loaded the software into an `msi` account. After logging into the user account, type the following command:

```
cat ~msi/biogv300/.setup300>>~/ .cshrc
```

This command adds two commands to your `.cshrc` file. One defines a pointer to the software directory. The other executes a shell script which defines some useful aliases and sets the environmental variables necessary to run the program.

- 8a) Alternatively, if you have chosen not to install the software in an `msi` account, you will need to edit your `.cshrc` file to include the lines shown below:

```
setenv MSIUSR /usr/your_directory_pathname
source $MSIUSR/biogv300/.setmsi300
```

substituting for "`/usr/your_directory_pathname`" the complete pathname of the directory in which you have installed the MSI software files.

- 9) If you have an earlier version of this MSI software, it is necessary to remove all old `setenv` and `alias` commands from your `.cshrc` file. In particular, please remove the command, `setenv BIOVER <version number>`, and any references to `BIOVER`. Also remove the command, `source /biograf/biogv${BIOVER}/bg_login.csh`, from your `.login` file.

- 10) Log out and then log in again so as to execute the new commands that you just entered into your `.cshrc` file. If there are command lines in your `.cshrc` file that the system doesn't understand, it will not finish the script and the aliases may not be defined.
- 11) Run the COMSTRUCT procedure by typing:

```
comstruct
```

COMSTRUCT allows you to configure the system to run the program in whatever way you choose. Select the program that you wish to run when asked to do so. Initially, it is easiest to hit only a carriage return in response to the questions in COMSTRUCT, selecting the default values. Later, when you better understand your preferred environment, you may customize your setup. Refer to the COMSTRUCT User's Guide, Appendix A in this document, for help as necessary.

You may use an alias of your own if you wish instead of the suggested default. However, if you use another alias or have COMSTRUCT place files in any directory other than your home directory, you will need to include an alias command in your `.cshrc` file so that the system recognizes your particular alias. Running COMSTRUCT generates a `.doc` file, the name of which is the alias you chose with `.doc` appended to it. The `.doc` file contains an alias command to include in the `.cshrc` file for non-default aliases or when using another default directory. If you change `.cshrc`, log out and back in again.

3.6 Running the Software

You should now be ready to run the MSI software. Before doing so, make sure that you have Xwindows running. If not, start it at this time by typing:

```
xinit
```

From the resulting window, you may run the desired MSI program by typing the alias you selected when you ran COMSTRUCT, *e.g.*:

```
biograf
```

To create additional configurations, run COMSTRUCT again as desired, selecting the necessary options to run the program in the way you choose. In order to execute the program in these new configurations using custom aliases, you must edit your `.cshrc` file to include the alias commands shown in the `.doc` files generated by COMSTRUCT. You may then safely delete the `.doc` files.

If upon starting the program, you receive an error message stating that there has been an authorization failure, please note the message and report it to MSI customer support. In most cases, such a message indicates that your software tape was made before your system id was known, resulting in an invalid authorization code.

You may obtain your system id by typing:

```
getsn
```

Report the output from `getsn` to MSI customer support, and they will send you the necessary changes that must be made to your authorization file. To make those changes, edit the file:

```
$MSIUSR/biogv300/exe/auth300.fil
```

Installation of the MSI program is now complete.

Appendix A

COMSTRUCT Users Guide

The COMSTRUCT program is used to create startup configuration files which setup and execute MSI software products (BIOGRAF, POLYGRAF, NMRgraf, or Polaris) with a specific graphics display, force field, and other defaults. COMSTRUCT configures a single product, hardware, and force field combination at a time. It produces three files: instructions for modifying your login procedure, a command file run to execute the product, and a startup defaults file. By choosing different option and command names, you may set up as many predefined configurations as you like or use COMSTRUCT as a query driven startup.

Upper case and lower case file names and commands are not equivalent. Thus, some data for COMSTRUCT is case dependent. When case is important, the program indicates this in the input prompt. In all other situations, the case of your responses does not matter. The command scripts produced by COMSTRUCT are designed to run in the "c" shell (csh).

A.1 Starting COMSTRUCT

Execute COMSTRUCT by typing construct at the command prompt:

```
construct
```

Next the copyright notice will be displayed, and you are asked whether or not you would like an introduction.

```
Would you like an introduction? ( [YES] NO )
```

Almost all responses have default values, marked by square brackets (*e.g.*, [YES]) and obtained by pressing "Return", or typing the string in brackets. When there are multiple choices listed, only the leading unique characters need to be typed. Replying with a question mark will produce further instructions, if available, or repeat the list of options.

For the most part, the COMSTRUCT input is self-explanatory. The remainder of this guide explains each COMSTRUCT query and shows typical examples. First, press "Return" to review the introduction.

A.2 Product Selection

Next users are asked to select a product:

```
Enter the product name: [BIOGRAF] POLYGRAF NMRgraf Polaris
```

Any product name listed may be entered, however only licensed products are available for execution. If you are not licensed for a MSI product, it may not appear in the list. After you type a selection (or "Return"), COMSTRUCT will echo your choice. For example, pressing return to get the default produces the following reply:

```
The product BIOGRAF will be configured.
```

All selections made by the user are verified in this way.

Note: This question is skipped for those that have licenses for only one MSI product. In this case, the system is automatically configured appropriately and a message is displayed indicating which product will be configured.

A.3 Graphics Display Selection

Next you are asked to select a graphics display device:

```
Enter the graphics device:
```

```
Workstation:          [type of host]
No graphics:          [None]
```

You have a choice between displaying the graphics window on the console or selecting no graphics at all. If you select no graphics, COMSTRUCT will generate a .def file containing the line:

```
L_BATCH          YES
```

When you run that configuration, the program will start up in command mode with no graphics display.

A.4 Force Field Selection

Next you are asked to enter the name of the force field to be used:

```
Enter the force field name: [DREIDING-II] DREIDING-I AMBER
                             AMBER-B MM2 MMP2 USER
```

Note: NMRgraf is supplied with the Dreiding-II force field only, hence only the DREIDING-II option appears in the prompt. NMRgraf users who wish to use Dreiding-I, AMBER, AMBER-B, MM2, MMP2, or the USER force field must obtain a BIOGRAF license.

At present, the program must be restarted to change force fields. However you can save your structures following a simulation with one force field, restart the program, and then use these same structures with another force field. Of course proper atom types must be present in each force field to represent the structure. Also, the energetics will change when the force field changes. See the *BIOGRAF Reference Manual* or the *NMRgraf Reference Manual* for a description of the force field options.

The USER force field allows local modifications to the parameter or conversion files to be incorporated into your standard configuration files. If you enter USER, you will be asked to type the names of both the parameter file and the conversion file:

The force field USER will be configured.

Enter the force field parameter file name, including the node or device and directory:
and

Enter the force field conversion file name, including the node or device and directory:

The standard parameter file are listed the table below. You may enter the file names as you would type a normal file name on your system, or you may use the environmental variable as shown. The file names are case sensitive. BG_EXE is an environment variable pointing to the standard force field directory. It is defined when you run the program.

Standard Force Field Parameter and Conversion Files	
Force Field	File Name
Dreiding-I	\${BG_EXE}dreidi300.par \${BG_EXE}dreidi300.cnv
Dreiding-II	\${BG_EXE}dreidii300.par \${BG_EXE}dreidii300.cnv
MM2	\${BG_EXE}mm2300.par \${BG_EXE}mm2300.cnv
MMP2	\${BG_EXE}mmp2300.par \${BG_EXE}mmp2300.cnv
AMBER	\${BG_EXE}amber300.par \${BG_EXE}amber300.cnv
AMBER-B	\${BG_EXE}amberb300.par \${BG_EXE}amberb300.cnv

A.5 Command Name Selection

The startup files created by COMSTRUCT create a command which invokes that particular configuration of the program. For VMS systems this will be a DCL global symbol, and for UNIX it will

be an alias. You are next asked to define the command name. For example, for BIOGRAF, the prompt will be:

```
What would you like to type to execute this configuration
of BIOGRAF? (case sensitive!) [biograf]
```

You will want to provide a unique name for each configuration, and one which can be easily remembered. The default is the name of the product selected (BIOGRAF, POLYGRAF, NMRgraf), which is adequate if you only run one configuration. Note that the command name is case sensitive.

A.6 Defining Startup File Names

Next you must define the names to be used for the files created by COMSTRUCT. This involves entering the directory (or logical name) and the prefix for the file names. First you are asked for the directory. The system will request:

```
Enter the name of the directory which will contain the files
created for this configuration. The default value shown
means your home (login) directory. Directory names are case
sensitive! : [${HOME}/]
```

Typically this would be your login directory (the default) or a public directory for all MSI software users. Next you are asked for the file name prefix, *e.g.*:

```
Enter a file name prefix for this configuration. Suffixes
and extensions will be added to create the final file names:
(case sensitive!) : [biograf]
```

This file name prefix may contain only characters legal in a file name. Do not include a directory or file name extension. It may include letters, digits, and any special characters allowed in file names. The maximum number of characters in the file name prefix is less than the maximum length of file names on your system because the name supplied will be extended with a suffix to make the final file names. The default file name prefix is the same as the command name previously entered.

Next the actual file names to be written will be listed, and you will be asked to verify that they are correct. For example:

```
Instructions for modifying your login procedure will be
written to:
```

```
  ${HOME}/biograf_cshrc.doc
```

```
The commands to be run at execution time will be written to:
```

```
  ${HOME}/biograf_run.csh
```

```
The startup defaults file will be written to:
    ${HOME}/biograf.def
```

```
Are these names OK? ( [YES] NO )
```

A NO response will branch back to the directory name query at the beginning of this subsection.

A.7 Including Defaults From Another File

COMSTRUCT creates a defaults file describing your graphics system. However, defaults files may include many other kinds of default settings. Essentially every default value which appears on a bottom menu in the MSI program can be set in your defaults file. All of the parameter names and their default values are given in the sample defaults file shown in Appendix D.

Rather than modify the defaults file created by COMSTRUCT, you may supply a secondary defaults file name. COMSTRUCT inserts a command at the end of the primary defaults file that processes the secondary defaults file. Thus, there can be a common set of COMSTRUCT configurations, but each user can still have his own set of defaults. You are asked:

```
Would you like to add defaults from another file?
( [NO] YES )
```

and if you reply YES, you must supply the file name. The request is:

```
Enter the supplementary defaults file name, including the
node or device and directory (case sensitive!) :
[${HOME}/standard.def]
```

Enter the supplementary defaults file name as you would specify any file name on your system. The default response lets every user have his own defaults file, called standard.def, in his login directory. If this file does not exist, a nonfatal warning will be printed at run time.

A.8 Startup File Creation

At this point all of the startup files are written, as indicated by the messages:

```
Creating command and defaults files...
Startup command construction is complete.
```

The files are now ready for installation, or you can continue on to run the selected product.

A.9 Immediate Execution Mode

In the final query, you are asked if you want to execute the specified configuration immediately:

Would you like to run this configuration now? ([NO] YES)

If the MSI program has been completely installed, then you can run a new configuration immediately by answering YES to this question. If the installation is not complete, environment variables called BIOVER, BG_BASE and BG_SCR will not be defined and execution will fail.