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AVIV®
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January 21, 1994

To all AVIV Data System customers:

Enclosed is the newest software version _____.
The software now works on IBM AT compatibles as well as IBM PC compatibles. Please note that the start up process, auto(xx).bat is different now. (Where xx is the software type, 14, 18, 60, etc.)

There is a new temperature control that adjusts the bath temperature to bring the thermometer temperature to the set point. It only works if the control mode is on. You can still calibrate the bath without worrying about offset when the mode is off.

The way the control works is that the program waits until the temperature is stable, it then adds the error to the bath set point to bring the thermometer temperature closer to the set point. This cycle repeats until the thermometer temperature is close enough.

As before you specify two parameters that are used to decide when the temperature is stable. These have new default values. We suggest that you leave them as set until you get some experience with the new system.

During the adjustment cycle the program uses the tight tolerance to decide if the temperature is close enough. Once the program sees that the temperature is stable and close enough it switches to the loose tolerance. The cycle will not restart unless the temperature deviates by as much as the loose tolerance.

When the temperature set point is changed the program uses a complex algorithm to adjust the new set point. The program tries to predict what the offset will be at the new temperature. Our experience so far shows that for small changes of temperature we arrive at the new set point after one adjustment to the initial offset guess to within 0.1 degree of the set temperature.

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The information shown at the top of the screen has been changed slightly. From left to right the fields are d, the temperature derivitive estimate, r, the remaining time intervals before we decide it is stable, b, the temperature sent to the bath, c, the bath temperature correction amount, a, the actual temperature, e, the error between actual and set temperature, t, the tolerance in effect, and four flags, ABCS, which indicate A, that the temperature is being adjusted, B, that a scan is about to begin and the program should wait 1 equilabration time whether the temperature changed or not, C, that a correction is about to be performed, S, that the error should not be added to the correction factor the next time the temperature is changed.

The control F7 key still gives you access to the control parameters. The default values as mentioned are all changed but they still work as described. The sampling interval is now every 6 seconds and we wait much longer to decide that the temperature is stable. You should be cautious about shortening the wait because the feedback system will become unstable if the delay is not long enough. The range of adjustment of the correction factor is limited to a few degrees around the temperature that the program thinks the offset should be. If the limit of this adjustment is reached the c label at the top of the screen will change to an L.

Obviously, if you break the feedback loop, by for instance removing the thermometer from the cell holder, the bath set point will drive to the limit.

There is a new program called DAC_INIT.COM . This program should be run as part of the autoexec.bat file on your instrument. Among other things this will insure that the bath set point is not disasterously high if you turn on the electronics but don't run the instrument program.

Try it we think you will like it.

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begin.doc - return to beginning mode

There is a control in instrument software versions starting with version 3.3i that allows the operator to choose whether or not the X axis variable is returned to its beginning value at the end of a scan.

In prior software versions wavelength mode always returned to the starting wavelength and temperature mode always stayed at the last temperature after a scan. Starting with version 3.3i the user can control whether the wavelength and/or the temperature stays at the last value or returns to the starting value. That is, this single choice now affects the behavior of both wavelength and temperature scan modes.

The convention chosen is that the instrument will always return to the beginning value by default. This decision leaves wavelength mode unchanged but reverses the usual end operation of temperature mode.

The operator can review and alter the current setting of this return-to-beginning mode state from the keyboard. To see the current setting press Control-PageDown. The program will present a list of control settings, one at a time. The last item in this list is the setting of whether the system will return to the beginning after a temperature or wave scan. There are two meaningful states for this setting, 0 or 1. A setting of 0 means DO NOT RETURN TO THE STARTING VALUE and a setting of 1 means DO RETURN TO THE STARTING VALUE. The operator can enter a new value if desired or can leave the current setting alone by just pressing ENTER. The state will remain as set until it is changed again or until the program is restarted.

The state of the return to beginning mode can also be altered from command files. There are two related commands available. One reverses the current setting and the other allows the state to be set directly on or off (1 or 0)

[TOGL_BEGIN_MD] This command reverses the current state of the return to beginning mode.

[SET_BEGIN_MD,1] This puts the instrument into the mode where it will return to the beginning after a wave or temperature scan. This is the default startup setting.

[SET_BEGIN_MD,0] This puts the instrument into the mode where it will will not change the wavelength or temperature after taking the last point of a scan. This used to be the operation of temperature mode. If desired this command could be included in the startup file, AUTOEXEC.AVI, to change the default setting.

Good control of sample temperature is essential to obtaining reproducible results for many users of Aviv spectrometers. We have been working to satisfy this customer need for several years now. Our cell holders are designed to accommodate standard 10mm path length cuvettes. At first the sample temperature was controlled by use of an external water bath. Control of the sample temperature was achieved by sensing water temperature near or in the sample and offsetting the bath temperature as needed through the bath remote programming interface.

This first temperature controlled cell holder, like its successors, included a magnetically coupled cell stirrer. Stirring is useful both to increase mechanical mixing and also to speed up temperature equilibration. Other important design features are provision of nitrogen purge ports to prevent condensation on cell windows, and spacers to allow the use of short path length cells (1, 2, and 5mm). The cell holders have ample depth to contain standard stoppered cells without producing heat leaks.

As our experience with temperature control accumulated it became evident that a faster means of changing temperature was desirable. The water bath presented other problems as well as being slow. For instance, it was difficult to isolate the instrument from the sample temperature changes. Also, high and low temperature plumbing is hard to do, and no ideal heat transfer fluid exists over the full temperature range that users wanted.

The response was to develop a thermoelectrically controlled cell holder. The thermoelectric cell holder is most noticeably faster than a water bath when the temperature is being lowered rapidly by a large amount, as it often is after a melting experiment. In this case the absence of the large mass of water makes a decided difference in time to reach temperature. Because the thermoelectric holder has room for water cooled heat sinks, the isolation between the sample temperature and the instrument is excellent. Because the heat sinks use water near room temperature, the plumbing problems are greatly reduced.

User needs for higher temperatures prompted us to change our thermometer measurement range from -50 to 100 degrees C to -50 to 125 degrees C. The standard controller has specified performance from -10 to 110 degrees C, with setting resolution to 0.1 degree, and can change temperature faster than 10 degrees per minute.

Although the thermoelectric controller can reach a selected temperature rapidly, sufficient time must be allowed for the sample itself to reach temperature. Sensing the actual sample temperature is not always possible, even though we do supply a teflon encased temperature sensor probe. With temperature controlled by a sensor just outside of the cell, we have provided for an empirical, approximately optimal speedup by allowing the user to program the thermoelectric holder temperature to deliberately overshoot for a short, controlled time, thus bringing the interior of the sample to temperature faster.

The instrument software supports several kinds of temperature related experiments. First, wavelength scans can be made with constant temperature control. Second, wavelength scans can be taken at a series of pre-programmed temperatures. In kinetics mode, temperature can be changed at will by the operator (or by program) to create temperature jumps. Temperature slew rates can be limited, if desired, to create temperature ramps at selected rates. Temperature can also be recorded as a function of time during these experiments. Finally, temperature can become the

independent variable and temperature scans (melts or freezes) can be performed. Up to 5 wavelengths can be followed during a temperature scan.

The thermoelectric device has proven easy to use and has become a popular accessory to our instruments. We are still in the process of developing variations of it to satisfy remaining needs. The first variation under development is a thermoelectrically controlled multiple cell holder. This device allows up to five samples to be studied at once, all in the same thermal environment. Besides reducing inter sample variation, the total time for a melting experiment is reduced because five samples can be equilibrating at a new temperature at once. A multiple cell holder is als effective in increasing instrument throughput when long kinetics experiments are being done at constant temperature.

Temperature Controls
  Shift F1 ... set setpoint temperature (need temperature controller)
  Shift F2 ... set temperature equilibration time delay (need controller)
  Shift F3 ... toggle temperature setpoint mode (prompt S) (need controlle
  Shift F4 ... toggle temperature recording mode (prompt T)
    (data recorded when temperature was controlled are tagged "TE")
Temperature Settling Controls (needed for special cases only - see notes)
  Ctrl F7 .... Temperature control sampling interval (decimal minutes).
               Temp. derivative tolerance for "stable" (deg C/interval).
               Extra derivative intervals beyond minimum 4 for "settled".
               Begin scan (tight) temp. tolerance (deg C).
               In scan (loose) temp. tolerance (deg C).
               Temp. error iir smoothing filter multiplier (per interval).
               Fraction of smoothed error to add to next target. (tracking)
  Temperature control offsets bath temperature to make thermometer read the specified temperature. If setpoint mode is off, Shift F1 allows direct control of bath setpoint with no correction. Correction range is limited to a small range about the expected offset.
Thermoelectric controls (appear on Ctrl F7 if thermoelectric installed)
      Set jacket overshoot temperature (deg C) (to hasten cell settling)
      Set jacket overshoot time (sec) (after which correct setpoint restore
      Choose thermometer temperature to show (j)acket, (p)robe, or (s)ink
      Set the maximum rate that setpoint will change at. (generate ramps)

Section 1 Introduction to AVIV Software

1.1 AVIV Software

Primarily, AVIV supplies software written by AVIV to operate the AVIV DS line of instruments. Miscellaneous software is included to enhance the usefulness of AVIV DS instruments. The PLOT program includes all features of the DS program, but allows user to operate plotters instead of an instrument (see table x for list of supported plotters). Batch files are included that automate certain aspects of instrument operation, and provide support for upgrading software.

AVIV supplies commercially available software that is of general use. The commercial software comes with detailed manuals, which should be consulted before using the software. The AVIV programs require the MS-DOS operating system, and MS-DOS and related files are included as part of the complete instrument system. An editor program is included as part of the system to aide in writing batch files, command files and examining data files.

AVIV can supply optional commercial software. Programming languages can be supplied to transform data sets and generate automatic reports. Programs to transfer data between different computer systems are also available.

There are several DS programs which operate different instruments. The instruments are divided up into four categories, two measurement techniques, and two monochromator types. Spectrophotometers measure absorption, transmission, and with special optional accessories reflectance. Circular dichroism spectrometers measure the difference in absorption between right and left circularly polarized light. AVIV uses double monochromators to increase optical performance. Double monochromators decrease stray light and increase resolution. The two monochromators are prism/grating and prism/prism. The model numbers for the various combinations is in table n.

The AVIV DS and PLOT programs share many features. The basic user interface is common to all programs. The programs share the same data structures, data file format, command language and data manipulation routines.

This Introduction to AVIV software covers the common features of the AVIV DS

and PLOT programs.

Table 1 Types of AVIV DS instruments

monochromator	technique	
	ABS/TRANS	CD
prism/grating	14DS, 14DS-IR 17DS, 17DS-IR	40DS, 41DS
prism/prism	118DS	60DS, 61DS, 62DS

1.2 Using AVIV software

The standard method of operating the AVIV software is from the keyboard of the system computer. The operator controls the software (and therefore the instrument) by pressing specific keys which instruct the software to perform specific functions. When a function has been invoked, the software often prompts the operator for additional information. Once the information is supplied the function is performed.

Standard abbreviations in the keyboard system **Ctrl, Shift, Alt** mean to HOLD DOWN the named shift key and tap the named key following. (i.e. there are 4 cases for some keys). "Toggle" controls alternate between two states (like on/off) and take effect immediately. Commands that take numeric values produce a prompt on the message line. The prompt gives the present value of the associated parameter and asks for a new value. You may enter a new value and press enter to change the value. Simply pressing enter leaves the value unchanged. Typing errors can be corrected by backspacing over mistakes.

The keyboard commands have descriptive names. By providing names for commands, sources other than the keyboard can operate the software. Commands can come from files stored in the local computer or from a remote computer through the serial port. The command system names are easier to remember, often self describing, and generally extend both software and instrument capabilities.

The original keyboard command system will be the operating system of choice for most users. However, even these users cannot totally ignore the command system. A command file (autoexec.avi for DS and autoexec.plt for PLOT) is read by the program as the program starts. This file provides information to customize the software or instrument to suit each individual users needs.

The keyboard is limited to about 100 commands, while the command system has the potential of an unlimited number of commands. For some instrument applications, the command system has definite advantages over the keyboard system. A second computer can be programed to control the instrument, allowing data collection and data analysis that are not supported in the basic instrument software. Unattended instrument operation during long experiments is possible with the command system. Simple repetitive tasks can be automated to free up human manpower for other duties. Command files can insure consistency of experimental details between different operators on different days.

The instrument can keep a log of all the commands it was asked to execute, from either the command system or the keyboard. Also, log files can record measurement. Communicating results and instrument status to a log file has proven very useful, especially in identifying problems. The logs, like all AVIV files, are kept in the standard ASCII form so that other programs can easily read them. Report generator programs are readily available that can read the instrument logs and extract results for use in subsequent analysis. In many cases the user can avoid having to write down and re-enter the information. On instrument start up a log is created in the instrument program subdirectory. This file operate.log contains all the commands issued during most recent instrument operation.

A detailed description of the command system is provided in another section of this manual. General discussions about the software use both the name and keyboard equivalent of each command.

1.3 AVIV programs and MS-DOS

The full name of a file includes a drive specification, a path specification and name of the file, including any extension. Detailed information about drives and paths is supplied in the MS-DOS manual.

1.3.1 Drives

The drive specification refers to the physical device that contains the file. The floppy drive in the current computer (AT&T 6300 or AT&T 6300 WGS) is device A:. The hard disk in the computer is device C:. Some computers have several drives, MS-DOS uses the letters A - E to designate drives. It is strongly recommended that data files be stored on floppy drives.

1.3.2 Paths

The path refers to the organization of a MS-DOS device. Every device has at least one directory known as the root directory. On drive A: the root directory is A:\. The hard drive is divided into many subdirectories, and MS-DOS needs to know which subdirectory to access to find a particular file. The 60DS programs are

located in the C:\C60 directory, the 14DS program is located in the C:\C14 directory, and the PLOT program is in C:\PLOT.

1.3.3 File names

File names in MS-DOS consist of up to 8 characters with an optional extension consisting of a period and up to 3 additional characters. Name extensions are used to distinguish broad categories of files, such as .bat for batch files. Use of extensions is completely optional, but you must be consistent, that is "scan" is a different file from "scan.ads". The full file name has the general form:

[DRIVE:][\PATH\]FILENAME[.EXT]

The items in square brackets are optional. No spaces are allowed in the file name. The acceptable set of characters for constructing file names is quite large and includes many punctuation characters, as well as letters and numbers. We recommend that you use punctuation sparingly. The colon (:), the backslash (\), and period (.) are reserved in MS-DOS and have special meanings. MS-DOS does not distinguish upper and lower case letters in file names, so scan.ads is the same file as SCAN.ADS. A partial list of useable characters is: A-Z, 0-9, !, #, $, %, (,), _, ', and -.

Program Startup

The DOS command "go 14" invokes the batch file go.bat, which passes control to auto14.bat. Auto14.bat is responsible for installing the memory resident parts of the instrument software and for managing the instrument power-on self test. Auto14.bat is reproduced below.

```
-------------------------------------------------------------
rem - this is auto14.bat
prompt $d $t$_$p $g
path c:\dos;c:\pe2;c:\;..
echo on
if %mr% == 1 goto trygra
set mr=1
rem - the following programs must run exactly once before starting 14ds
oitest
if errorlevel 1 goto exit
timer
multi
motor
if errorlevel 1 goto exit
servo
sample
:trygra
```

```
if %gr% == 1 goto tryrun
set gr=1
rem 0 0 oki; 0 1 epson, 0 2 tally (as lpt1)
graphics 0 0
:tryrun
14ds
:exit
```

The environment variables "mr" and "gr" are used to control the loading of the memory resident programs. Since the screen dump program can be loaded either by starting the instrument or by starting the plot program, a separate variable, gr, is used to indicate that the screen dump has been loaded. Both mr and gr are set to zero upon system boot by the autoexec.bat file in the root directory. When the resident programs are loaded the associated variable is set to 1 so that loading will not be attempted on subsequent go commands.

Power on self test is performed by the programs oitest.com and motor.com, which are run once as part of the instrument startup process. A failing program returns an errorlevel of 1 instead of zero. The batch file above detects the failure return and skips out of the startup process. Passing these two tests indicates that at least the core of the instrument electronics is working. This knowledge greatly simplifies problem diagnosis.

If a failure should occur, check first that the instrument electronics is powered on, and then reboot the computer to try the startup again. If a test repeatedly fails you should save the program output and call for help in interpreting the error messages. You can get a printout of the failing startup by setting DOS to copy to the printer everything sent to the screen. Hold the Ctrl key while pressing PrtSc to turn on this mode. Be sure that the printer is on and selected. Repeat the Ctrl-PrtSc to turn printing off again later.

Oitest.com checks the instrument interface data path inside the computer. Once this is known to work motor.com can check the data path into the electronics in the instrument. Once the digital data path is known good motor.com checks the behavior of the D/A - A/D converter pair on the instrument controller card. If the A/D converter checks good then erroneous values on the control screen can confidently be interpreted as failures in more peripheral circuits. These failures are extremely rare, but this procedure should result in more rapid diagnosis and correction of those that occur.

The list below shows the files normally present in the c:\c14 directory.

```
AUTO14      BAT     417  1-12-84   5:49a
```

```
AUTOEXEC AVI     297  8-02-88  11:37a
KEYS     LST   12912  9-21-87   8:33p
TIMER    COM      87  9-21-87   8:33p
MULTI    COM    1730  7-18-88   8:50p
MOTOR    COM    4062  7-19-88   9:19p
SAMPLE   COM   32979  9-21-87   8:33p
SERVO    EXE    6116  9-21-87   8:33p
GRAPHICS COM   17202  9-21-87   8:33p
HISTO    EXE   27910  9-21-87   8:33p
OITEST   COM    1914  6-10-88   6:47p
14DS     EXE  161613  7-19-88   9:05p
```

Oitest.com is a test program only, it is part of the power-on self test. Motor.com is a resident program that also performs part of the self test. Timer.com, sample.com, multi.com, and servo.exe are resident programs that perform various parts of the instrument function. The operation of these resident programs is not visible directly at the user level.

Graphics.com performs the graphics screen dumps. It may also be loaded as part of the plot program startup.

14DS.EXE is the main instrument program. This program collects and formats the data and manages the control screen. 14DS is not resident. Autoexec.avi is the first command file for 14ds. This file contains the startup profile for the instrument program. Autoexec.avi is a plain ASCII file that can be modified with any convenient editor to accommodate the instrument to the users preferred mode of operation. A separate section of this manual provides a complete reference for the commands available.

Here is the standard version of autoexec.avi.

```
/* autoexec.avi */
[PATH_LOG,"C:\C14\LOG\"]          /* where log files go */
[OPEN_LOG,"OPERATE.LOG"]            /* start the first log file */
[PATH_COMD,"C:\AVI\"]             /* where command files are located */
[PATH_DATA,"A:\"]                /* where data is stored */
[PATH_HELP,"C:\C14\"]             /* where the help file, keys.lst, is */
[EXECUTE,"C:\AVI\WAVECAL.AVI"]    /* set the home wavelength */
[WAVE_ULIM,800]           /* set hard upper limit */
[WAVE_LLIM,180]           /* set hard lower limit */
[SET_RIGHT,400]           /* set screen right limit */
[SET_LEFT,200]            /* set screen left limit */
[HOME_ALL,"Y"]                 /* home the monochromator */
[SET_TEMP,25]             /* set bath setpoint */
```

```
[REPAINT]                /* draw the initial screen */
[MAKE_SETUP]             /* make the first setup file */
-------------------------------------------------------------
```

The file "c:\avi\wavecal.avi" contains the wavelength calibration value for the monochromator. The program "INST-CAL.EXE" is provided to help maintain wavecal.avi. Inst-cal can be invoked from the DOS prompt. The only mandatory commands in autoexec.avi besides execution of wavecal.avi are [HOME_ALL,"Y"] to home the monochromator, [REPAINT] to draw the initial screen, and [MAKE_SETUP] to create the first instance of the special setup file.

Keys.lst is the file displayed by the key combination Alt-H [HELP]. The instrument program displays keys.lst 23 lines at a time. The standard file presents a short list of commonly used keys followed by a complete list of all keys grouped by function. Keys.lst is a plain ASCII file. You may modify this file as needed to present the information you find most helpful.

Histo.exe is a specialized program used to test and calibrate the A/D converter and attached circuits. Histo.exe is present for service use only. Histo can be run anytime after 14ds.exe has run once.

1.4 DS Programs

The DS program begins, after taking care of the self calibration procedure outlined above, by showing the DS program screen (Figure X). This screen is the basic screen used by all AVIV DS programs. The screen has reserved areas for the display of collected data, data collection parameters, current instrument status, and for dialogue between operator and program. Other screens are used to display disk directory listing, or a list of command keys. The Plot screen is very similar, however, there is no instrument status to display.

1.4.1 Graph Area

The most prominent feature of the DS screen is a large rectangle that takes up the lower right portion of the screen. This is the area used by the program to graph data (figure). The data points are graphed as dots. When several points are in the same screen pixel column, by default the program will average these values and display only one point. All of the data points can be shown individually by the command **TOGL_ALL_DATA (Alt 9)**.

1.4.2 Scan and Graph Parameters

Across the top of the screen are 7 lines of text which give information about how the instrument is (or was) set to collect data. This information is stored in the data file as the data set header. The first line is used to display error and alert messages

to the operator. The second line has the software version number and ends with system date and time. The third line starts with the creation date and time. The fourth line begins with scan information and ends with filename. The fifth line starts with the y scaling parameters and ends with motion status or program status. Line 6 is the note line and line 7 is the message/prompt line. The content of most lines can vary depending on the setup of the instrument and will be described in the appropriate section.

1.4.3 Program Dialogue

The first or error line is used to alert the operator of possible instrument problems. The error message is printed above the scan parameters to make it easier to find, errors are accompanied by a beep. Most errors require the operator to press <enter>, which signifies that the operator has seen the error. Sometimes the error is really an information messages rather than an true error.

The message/prompt line is used to input information to the program. Many instrument setting operations require numeric values (e.g. Going to a new wavelength). Most of these input routines give a short message and the current value, then ask for a new value. The new value can be typed in, or if the value is correct only <enter> must be pressed. Typing errors can be erased by backspacing

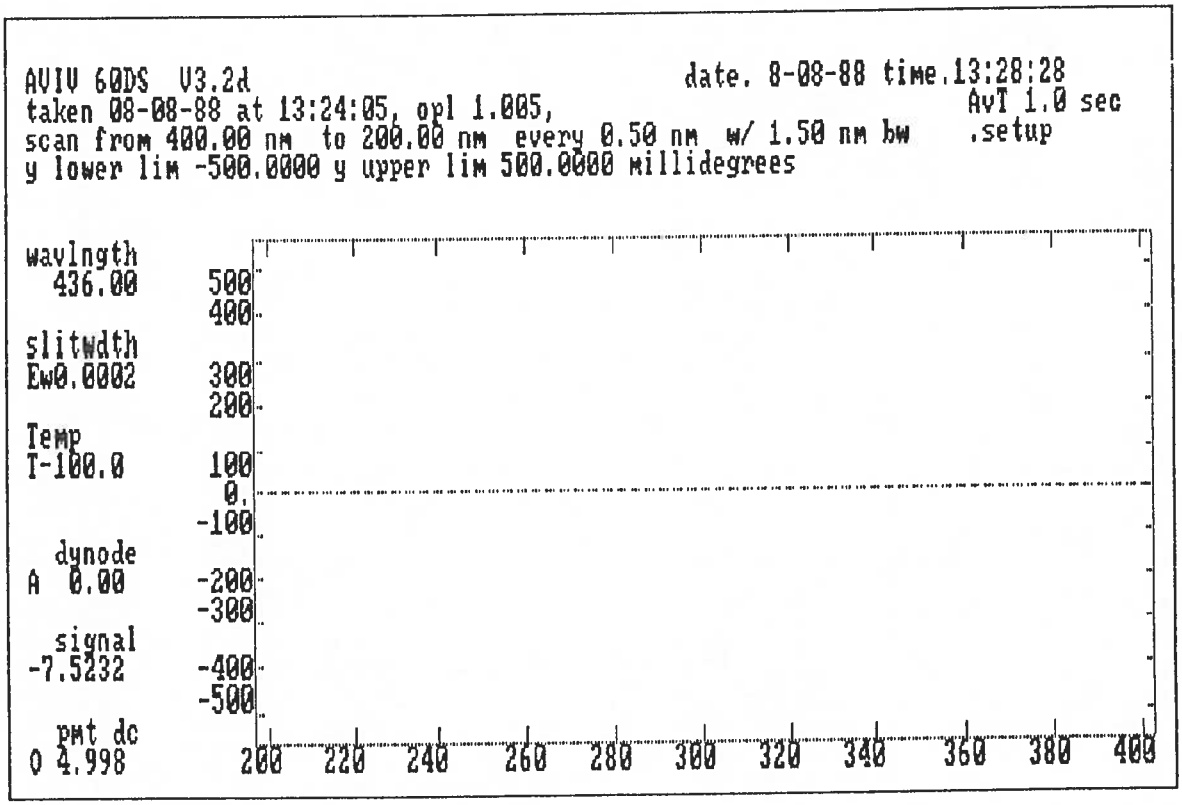

Figure 1 Example of AVIV screen.

over the error.

1.4.4 Graph Limits & Recording Limits

The data is presented graphically on the monitor, and the axes of the graph can be shifted and scaled as desired. For data collection the X axis can be in nanometers, second, or degrees Centigrade. The Y axis is in millidegrees for CD and either Absorbance or percent transmittance for spectrophotometers. The graph X axis limits set the data collection range. The Y axis limits only apply to graphing the data and do not influence the range of values that are recorded. The actual measured signal is determined by hardware, regardless of whether or not it will fit on the display.

The 4 graph extrema are displayed on lines 4 and 5 of the header. These parameters are updated as the graph limits are changed. The cursor keys are used to adjust the graphing parameters. To use the cursor keys Num Lock should be off (light off), pressing an arrow key will produce a prompt on the message line, giving the operator the option of changing the parameter. The four arrows are well described by their command system names: **RIGHT = SET_RIGHT, LEFT = SET_LEFT, UP = SET_UPPER**, and **DOWN = SET_LOWER**.

1.4.5 Redrawing the Screen

After changing graph parameters the graph is not redrawn until you tell the program to redraw the graph. **HOME (REPLOT)** uses the parameters shown in the data set header to redraw the graph. **END (FIT_Y)** uses the existing x scale, but adjusts the Y scale to make all of the data visible. **CTRL HOME (FIT_XY)** adjusts both the X and Y scales so all of the data is displayed.

1.4.6 Time-Stamping

Each data set is time-stamped upon creation. On screen this information is written on line 3 as "taken -date- at -time- ." The time and date of creation is saved as part of the data set header. The creation date and time can not be modified and is useful in determining when a data set was collected or last modified.

Do not confuse the creation date and time with the current date and time. The current system date and time, including seconds is the constantly changing display at the end of line 2.

1.4.7 Notes in Data Sets

To enter a comment or note to be associated with a data set both on screen and in the data file use **ALT N (NOTE)**. The program will prompt "n:" at the beginning of the message/prompt line. The user types any ASCII characters as the note and

presses <enter>, then the program shifts the text to the note line. To blank an existing note, the user should type a space as the note.

1.5 File Management

1.5.1 Drives and Paths

The default path for data, while in the Aviv DS program, is usually the root directory of drive A: (ie A:\). To change the default path, use **DEFAULT_DRIVE (Shift F8)**. The program will show the current data path and prompt for a new path. If you want to change the path enter a valid MS-DOS path (e.g. C:\DATA\). Alternately the default path could be set in the autoexec.avi file.

The paths the program will use to locate information should also be specified in the autoexec.avi file. Four different path designations should be included: 1) the location used to output a log file (**PATH_LOG**), 2) the path for command files (**PATH_COMD**), 3) the path to save and load data files (**PATH_DATA**), and 4) the path to look for the online help file KEYS.LST (**PATH_HELP**). The defaults for these paths are, respectively, the instrument directory, c:\avi, a:\, and the instrument directory.

1.5.2 Renaming a Data Set

The current data set can be renamed by using **RENAME (Alt R)**. A prompt will appear asking for a new file name. Type the name following the guidelines for a valid MS-DOS filename and press enter. The new name will replace the old name on the right edge of line 4 of the screen data header. A file may be renamed as many times as desired.

1.5.3 Data Sets in Memory

The program uses RAM computer memory very efficiently. Many data sets can be in memory at any time, as configured from the factory at least 50,000 data points can fit in memory. The data sets in memory are organized in a large ring. Each data set has two other data sets next to it. To move between data sets use **PRIOR (PGUP)** and **NEXT (PGDN)** to go around the ring. It is also possible to go directly to a data set by using **SHOW_DATA (Alt G)**. However, this requires the name of the data set.

As of version 3.21 a short cut has been introduced to help navigate data in memory. The command ????? **(F8)** will now put the names and some information about files in the ring on the message line. The same commands are used to move between data sets **PRIOR (PGUP)** and **NEXT (PGDN)**. This speeds up moving around the ring by not having to redraw each data set, which can be slow with many data points. The

information shown about each data set is the name of the data set, whether the data set is tagged, if the data set is in the plot list, and whether the file has been saved.

1.5.4 Saving a Data Set

Usually data sets are stored on floppy disks for future use. To save a data set use **SAVE_FILE (Alt S)**. The current data set will be written to disk under the file name shown on screen. Data files should be given unique names before they are saved on disk, because of the possibility of overwriting a file with the same name. The program will issue the warning message: "scan.ads is already on disk, OK to overwrite it? Type y or n." Typing n will abort the save.

1.5.5 Loading a Data From Disk

Use **LOAD_FILE (Alt L)** to load a data set. The operator will be prompted: "data set to load:" on the message/prompt line. Any saved data file can be loaded from a disk, if you know the name of the data file. To determine what files are on disk, you can have the program give a directory listing.

1.5.6 Disk file directory listing

To see a directory listing of files on any drive use **DIRECTORY (Shift F9)**. The program will then clear the screen and ask the user to enter a directory specification. The user should then enter: the drive designator, the path, and a file specification. Files can be specified by name or by the wild card characters: "*" and "?". "?" specifies a single letter, while "*" matches almost everything. Examples are given in table NN. The directory listing also shows any subdirectories.

1.5.7 Deleting a Data Set From Memory

To remove a data set from memory, locate the file, and use **REMOVE (Alt D)**. If the data set has not been saved, the program asks for confirmation before destroying it. You cannot delete the special file .setup.

Table 2 Examples of Directory Specifications

directory specification	action
a:*.*	- list directory of all files on drive A:
c:\	- list root directory of drive C:
c:\data	- list directory of subdirectory data on drive C:
b:*.ads	- list all files on drive b: with extension .ads
c60b.*	- list all files with name c60b and any extension
c*.?	- names which start with c and have one letter extension

1.5.8 Data File Format

Data sets saved as disk files are in the form of simple lists of data points, together with a header documenting the conditions under which the data set was collected. The files are in ASCII and can be examined on the screen using a text editor or alternately using MS-DOS copy or print utilities. The only items required by the AVIV programs to load a data set are: 1) that x_decr or x_incr precede the data, 2) that data lines should begin with either a digit, decimal point or minus, 3) header lines should begin with a non-number.

The header consists of an unknown number of lines with the usual form, keyword (space or spaces) value. The header information need not be in any specific order. A listing of keywords and some potential values are listed in the appendix. However, the user can modify both the x and y unit, either by performing a data manipulation, or by entering a different value. Header lines not including a keyword are ignored.

Keywords used in AVIV DS data files

Keyword	Value	
x_unit	seconds	
	degrees_C	
	nanometers	
	Angstroms	internally converted to nanometers
	unknown	
y_unit	%transmission	used in spectrophotometers only
	Absorbance_U	used in spectrophotometers only
	ellipticity	used in CD only
	millidegrees	used in CD only
	degrees_C	
	volts	
	microamps_x2	
	seconds	
	millimeters	
	deltaAbsorb	used in CD only
	unknown	
_y_type_	transmission	used in spectrophotometers only
	absorbance	used in spectrophotometers only
	ellipticity	used in CD only

	millidegrees	used in CD only
	temperature	
	dynode_volt	
	op_level	used in CD only
	ref_level	used in spectrophotometers only
	run_time	
	extern_data	
	unknown	
	slit_width	
	CircularDich	used in CD only
data_name	valid MS-DOS filename, optionally with drive and path	

notes:	up to 78 character text note
date	creation date (mm-dd-yyyy)
time	creation time hh:mm:ss in 24 time
temperature	creation temperature of data set in degC
wavelength	wavelength where data set collected in time or temp
repeats	number of repeats in Repetitive Scanning mode (integer)
delay	time (integer minutes) between starting scans in Repetitive Scanning mode
_temp_flag_	
_equil_time_	time (decimal minutes) for sample to settle in temp mode

With the following keywords only one of each set is allowed in any data set

Instrument operating level

reflevel	voltage in spectrophotometers only (usually about 7.00 volts)
oplevel	in CD only (usually about 1.005 volts)

Slit width control modes

dynovolt	voltage in constant energy mode (0 to 1000 volts)
bandwidth	spectral bandwidth in constant bandwidth mode (0.01 to 12.00 nm)

Time used to collect a data point

__avg__time__	used in wavelength and temperature modes time in seconds
__time-constant__	used in kinetics mode time in seconds

Step sizes in data collection modes

scan__step	step size in wavelength mode
time__step	step size in kinetics mode
__temp__step	step size in temperature mode

All three have same units as x__unit and should match spacing of x values in data

The following keywords do not have values associated with them

these keywords mark the beginning and end of the data in a data set

__data__
__data__end__

these mark the direction of the x values in the data set: wavelength scans always decrease, time scans always increase, and temperature scans can be either

x__incr
x__decr

the data set was baseline corrected only in wavelength mode

corrected

these keywords mark the beginning and end of a comment, which is ignored by the instrument and Plot programs

comm
endcomm

Data Formatting

The formatting of data in the data file depends on the units of collection. The following table details most of the formats. The format is X.Yf, which means a total of X digits with Y decimal places printed as a floating point number. The format characters d implies decimal and g implies floating point which switches to scientific notation when the field is exceeded.

Formatting Y values

y unit	y Type	abbrev	format
%_transmiss	transmission	%T	6.4f
Absorbance_U	absorbance	AU	7.6f
ellipticity	ellipticity	elip	7.6f
millidegrees	millidegrees	mDeg	5.3f
degrees_C	temperature	degC	5.3f
volts	dynode_volt	V	5.3f
microamp_x2	op_level	uA*2	6.4f
volts	ref_level	V	6.4f
seconds	run_time	sec	3.1f
volts	extern_data	V	6.4f
unknown	unknown	y	7.6f
millimeters	slit_width	mm	5.3f
deltaAbsorb	CircularDich	dA	5.3f

Formatting X values

x unit	x type	abbrev	format
nanometers	wavelength	nm	7.2f
degrees_C	temperature	degC	7.1f
seconds	time	sec	7.1f
Angstrom	wavelength	Ang	5d
unknown	unknown	y	7.6g

The unit abbreviations are used in data manipulations to create new units.

mDeg*2	millidegrees times 2
log(V)	log of voltage
millidegrees/nm	first derivative
AU/nm^2	second derivative

Section 2 Plot Program

2.1 Introduction
2.2 Autoexec.plt

A discussion is needed about the directories in which plot looks for specific information.

The file Autoexec.plt is read by the Plot program on startup. This file contains the setup information the program needs to work with your plotter. The following shows a listing of an autoexec.plt file. text enclosed between the /* and */ characters are comments. This file sets the paths the program will use: 1) to output a log file (**PATH_LOG**), 2) to look for command files (**PATH_COMD**), 3) to save and load data files (**PATH_DATA**), and 4) to look for the online help file KEYS.LST (**PATH_HELP**). Two different commands can be used to open log files: **OPEN_LOG** which overwrites the contents of a log file and **APPEND_LOG** which adds information to an existing log file. Both commands will create a new log file if none exists with that name. **CLOSE_LOG** causes the program to stop writing to a log. The **PLOT_TYPE** command sets the type of plotter the program expects (see table of supported plotters above). The **PLOT_PORT** command is used to select different serial ports if there are more than one. However, at present the Plot program is limited to using com1, which is port 0.

2.3 Plot Operation

If you are planning to run the Plot program on a separate PC you should run the AVIV graphics.com program first if you expect to take screen dumps on a printer. Please note the hardware the other PC must have, as listed in Basic system requirements above. Floppy disk users will normally start the Plot program by typing `pl <enter>` at the DOS prompt. Hard disk based instrument users will simply type `go plot <enter>`.

To start the Plot program you simply type `pl <enter>`. If you have a hard disk based instrument system, you can type `go plot <enter>` from any directory to start the plotter. The Plot program can also be started by typing plot in the directory where the program is located (usually c:\plot).

The program will start with the screen looking similar to the AVIV DS program screen. If the plotter is turned on the pen will be moved to the plotter origin. If

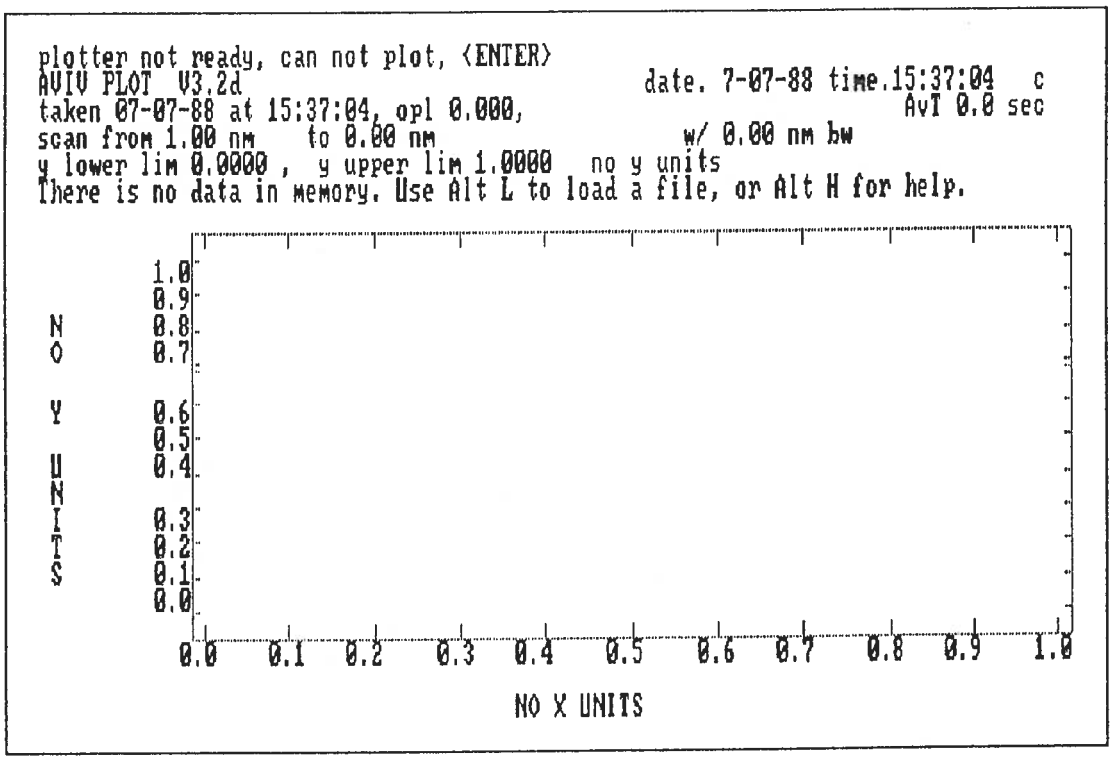

Figure 2 Plot program Screen

the plotter is not ready the program will present a message on startup. You can ignore this message and turn the plotter on later when you are ready to plot. Then, the user will be prompted for the name of a data file to load into memory.

The commands available with the Plot program are similar to the AVIV DS spectrometer programs. Commands that have to do with data collection are not included, and plotting specific keys have been supplied. The commands can be accessed in two manners: directly from the keyboard and from command files.

```
rem pl.bat
rem set up and run the plotter-screen program for the rem
HP 7440 plotter
rem these are the defaults, they do not need to be set
if not exist c:\needgrap.res goto tryrun
del c:\needgrap.res
rem 0 0 oki; 0 1 epson, 0 2 tally (as lpt1)
graphics 0 0
:tryrun
plot
```

Text of pl.bat

Keyboard commands are entered by pressing specific keys. Often commands require holding down one key and tapping a second key. For example, **Ctrl F1**, means to hold down the **Ctrl** (control) key and to tap **F1**. The complete list of available keys is an appendix to this document. The key list is also available on screen while the program is running by typing Alt H for help.

The command system should be described.

2.4 Plot Specific Commands

To plot the data set that is currently on the screen. Once this data set is ready to plot (assuming that the plotter is ready), **Ctrl F1**. This will start the plotting process.

Before actual drawing begins, the program will display the first pen choice. You may accept this choice or override it with any other valid pen number. When you press <enter> the plotter will start drawing. The graph border and text area are drawn first, then, if there is more than one pen, the program will stop and present the next pen choice. Again, you may accept or override this choice. When you press <enter> again the program will plot the data. If you need to stop a plot once plotting has started simply type **Ctrl F2**. The plotter may run on a bit to clear data from its buffer, but the program will not send any more information.

If you choose one of the overlay modes the program, will prompt you for a file name, then will plot only the data of the selected file, not the graph border or text information. **Ctrl F3** plots the selected data set using the scale of the current screen (like **Alt Z**). **Ctrl F4** plots the selected data set using the view of the selected data set (like **Alt X**). Either overlay mode can be used to plot a data set without borders.

Pen choice cycles through all the valid possibilities (default is the maximum number of pens possible for the plotter). The number of pens can be changed with the **Ctrl F5** key to reflect the actual number of pens available. The program can be told not to ask for confirmation at each pen change by using the **Ctrl F6** key. In the no-ask mode the program will only ask upon the start of a plot by **Ctrl F1**, the program will make all further pen changes on its own. The program will not ask at all in response to **Ctrl F3** or **Ctrl F4**. The next pen the program will use can be examined and changed by use of the **Ctrl F8** key.

On plotters that support automatic paper feeding, a new sheet can be loaded by the **Ctl F7** key.

2.5 General Plotting Suggestions

Two different screen graphs are possible: normal and full screen. The normal screen is where the data collection information is placed above the data graph. The full screen graph is where most of the text has been suppressed. Many people prefer

the full screen for presentations. The user can toggle between modes by use of the **Alt =** key. To suppress the file name you can rename the data set ".".

The full screen mode has the advantage of speedier plots. A second line of text is available only in this mode. This text is entered with the **Alt -** key. The same line of text is shared by all data sets in memory, so that it acts like a global heading line. The note lines can be blanked by entering a single space in response to the n: and n2: prompts.

Sometimes plots can be enhanced by changing the units on the axis labels. This is useful after complicated data manipulations, such that the graph can reflect the appropriate units. The Y axis can be relabelled by use of the **Alt Y** key. The X axis can be relabelled by first executing **Alt 3**, which switches the function of **Alt Y** (and several other keys) to work on the X axis. The Plot program is a little less restrictive about X axis units, since choices here cannot affect the data collection process.

A zero reference line can be turned on with the **Alt 0** key. This line will normally plot in a different color. The line will be displayed on any graph where zero is part of the Y axis range.

The Plot program will plot wavelengths in nanometers regardless of whether the data was recorded in nanometers or in Angstroms. Some data collected on CDs with previous software versions will be in Angstroms. To load kinetics or temperature data correctly that was recorded in Angstroms you will have to use the **Alt F3** key to tell the program to assume that the recording wavelength and bandwidth are in Angstroms.

When plotting, a line is drawn to every recorded point. You can get a better preview of this effect on screen by using the **Alt 9** key to switch to the show-all-points mode of screen display. Normally the screen is drawn with no more than one dot per possible x position by plotting the average of all points that map to the same column on the screen. This is faster and usually clearer.

Section 3 Data Reduction/Data Manipulations

3.1 Introduction

The DS programs and Plot share a diverse set of routines to manipulate data. These routines range from simple mathematical operations (addition and subtraction) to complicated data set transforms.

To extend the number of possible keyboard operations we have chosen to put x axis operations on the same keys as the corresponding y axis operations by assigning a temporary shift key (**Alt 3** or **TOGL_X_NEXT**) to select an x axis operation. Each time you press **Alt 3** the x selection state will toggle, press it once to select an x axis operation, press it again to switch back to y axis mode if you decide not to perform an x axis operation. Performing an x axis operation switches the x selection state off again, so the **Alt 3** key must be pressed once before each x axis operation. This kind of operation should be familiar to most users as many scientific pocket calculators use a similar scheme.

3.2 Baseline Correction

Baseline correction is especially needed in a single beam instrument like the CD. The baseline can correct for deviations in either the cell or in instrument baseline response. Note that a baseline scan should match the spectrum to be corrected in terms of wavelength range and spectral resolution. However, if they do not contain all the same points the result will contain only the points that did match.

3.2.1 Baseline designation

One spectrum in memory may be designated the baseline spectrum by typing **Alt B** (**BASELINE**) while displaying that spectrum. Any pre-existing baseline designation is automatically removed. A reminder letter, B, will appear near the file name of the designated baseline spectrum while it is on screen. A lower case b will appear on other data files to signify that a baseline has been selected.

3.2.2 Baseline correction

Once a suitable baseline is designated, baseline correction may be applied to a similar spectrum by displaying that spectrum and typing **Alt C** (**CORRECT**). This process creates a new data set, which has the same name as the original data set, but the

extension, ".acd" . If a corrected spectrum of the same name already exists in memory then the program will fail to correct the file. The program remembers that a baseline correction has been done and will not allow a second correction. That a spectrum has been corrected is stored in the data file on disk.

3.3 Simple Mathematical Operations

3.3.1 Operations with constants

3.3.1.1 Multiply a data set by a constant

To multiply the current data set by a constant use **MULTIPLY (Alt M)**. The program will ask the user to enter a number which is multiplied by each Y value in the data set. This results in a new data set with the same name but with extension ".mul". (**Alt 3**) Multiply each x value by a constant.

3.3.1.2 Add a constant offset to a data set

To add a constant offset to the current data set use **OFFSET (Alt O)**. The program asks the user to enter a number to be added to each point in the data set. This results in a new data set offset from the original with the same name but with extension ".add".

(**Alt 3**) Add a constant to each x value (compensate for spectral shift).

3.3.1.3 Divide a data set by a constant.

To divide the y value of each point in a data set by a constant (point/constant) use **DIVIDE (Alt 5)**. The program will prompt for the constant to use. This results in a new data set with the same name and the extension "div".

To divide each x value by a constant use (**Alt 3**) before issuing the command.

3.3.1.4 Inverse of a data set.

To take the inverse of a data set use **INVERSE (Alt V)**. This command performs the following operation constant/point. The program will prompt for the constant. This results in a new file with the extension "inv".

use (**Alt 3**) before the command to Divide each x value into a constant. This is useful because it can convert nanometers to wavenumbers (cm^{-1}).

3.3.2 Operations between data sets

Two data sets can be combined in an operation, such as data set subtraction, even if they do not contain all the same points. The result will contain only the points that did match. This can be described as the intersection of the two data sets.

3.3.2.1 Summing two data sets together

To sum two data sets use **ADD (Alt P)**. The program will ask the user to enter the name of the data set to be added to the current data set. A new sum data set will be created with the name of the current data set and extension ".sum".

3.3.2.2 Subtract one data set from another

To subtract a data set from the current data set use **SUBTRACT (Alt Q)**. The program will ask the user to enter the name of the data set to be subtracted from the current set. It will produce the result data set with the name of the current data set and extension ".dif".

3.3.2.3 Weight of 2 data sets.

WEIGHT
Alt E weight this data set with another data set
filename *.wei

3.3.2.4 Ratio of 2 data sets.

RATIO
Alt 6 ratio this data set with another data set
filename *.

3.4 Complex Mathematical Operations

3.4.1 Smoothing

SMOOTH
Alt I does the smoothing and **Alt 7** sets up the parameters.
Filename *.smo
some learning effort will be required to develop the judgement to make good choices easily in smoothing parameters.
Smooth by least squares polynomial fit up to 10th order, 125 points. (Also includes a test of the randomness of the changes, which checks the reasonability of the smoothing.) (Also takes up to 9th derivative of data - depending on the polynomial used.)

The smoothing operation involves the least squares fit of a selected polynomial to the original data in a window around each point. The original point value is replaced by the value of the polynomial at that point. The least squares coefficients are correctly calculated for the non-centered windows necessary at the ends of the data range. The polynomial order and window size to use are both selectable. In addition, the derivative of the polynomial at the point (of any degree up to the order of the polynomial) can be selected instead of the value of the polynomial itself.

A statistical test of the fit is also available. This test is based on the notion that the differences between the smoothed and original data ought to be random if the polynomial is a good estimate of the underlying true data. (That is, the differences would mostly consist of random noise.) The randomness of the differences can be tested be comparing two estimates of their variance. The conventional estimate of variance, s^2, the mean square difference, is independent of the order in which the differences occur. A second estimate of variance, the mean square successive difference, d^2, is very much dependent on the order in which the differences occur. The ratio of these two estimates should be 2 if the differences are truly random. An improbably low value indicates some long term trend in the data, roughly speaking, over smoothing, while an improbably high ratio indicates short period oscillations, perhaps due to using too high a polynomial order or too small a window. The ratio is presented along with 5% and 1% probability limits. A ratio outside the 1% limits indicates that there is little chance that the differences were actually randomly distributed. This test is suggested as a guide to determining good choices for the polynomial order and window size. Optimal values by this criterion change considerably depending on the data being fit. You can look at the actual differences between the original and the smoothed data by using the data set subtraction operation. You can also suppress the statistical test if you don't like it.

3.4.2 Peak Picking

PEAK_PICK
Alt J does peak picking and **Alt 8** sets up parameters
filename *.pks
Locate extreme points (peaks) in a data set. (Uses smoothing & derivative)
The peak picking process builds on this smoothing and differentiation capability as a base. The peaks are determined by first creating a smoothed data set and a (smoothed) first derivative data set. (The polynomial and window parameters for each operation, smoothing and derivatization, are chosen separately. We are not sure if using different choices for the two is ever a good idea, but we thought some user might want to.) The derivative set is then scanned to find zero crossings of slope appropriate to an extreme point. The height of the detected extremum is then compared to two threshold criteria, those that pass are placed in the peak data set.

There is a global threshold based on the absolute peak height and a local threshold based on the peak height relative to the nearest valley point. The local threshold is

always expressed as a percentage of the total y axis range. The global threshold definition varies slightly depending on whether the y range includes zero. If the y data range includes zero then there are two global thresholds, one for positive peaks as a percentage of the highest positive peak relative to zero, and a similar, separate one for negative peaks. If the y range is unipolar then the global threshold is based on a percentage of the total y range, and is compared to the y limit closest to zero. Certainly other definitions of peaks are possible, and we would appreciate suggestions of any that seem useful.

When a peak is found the program will either return the smoothed y value corresponding to the derivative value closest to zero, and that x value, or it will do a linear interpolation of the derivative x value to find the exact zero crossing and add the area of the triangle determined by the zero crossing and the nearby x point (the approximate integral of the derivative) to the smoothed y value to make a better estimate of the peak height. In this mode the program will report peak locations to .01 nm. Which method is used is under user control. Switches are also available to control whether to perform the d 2/s 2 test during the smoothing, and whether to keep the smoothed and derivative data sets used to pick the peaks.

The list of peak pick parameters is long right now. We expect to simplify access to the rapidly multiplying list of user accessible parameters and functions in a later release this year. It seemed better to get the functionality out now however so that those that really need it can start to use it.

3.4.3 Derivatives

SMOOTH
SMOO_DERIV,1
Part of **Alt I**
filename *.d2w for 2nd derivative of wavelength

3.4.4 Transforms

3.4.4.1 Add a constant to $\log_{10}$ of each point.

LOG
Alt U takes the $\log_{10}$ of the current data set
Filename *.log
(Alt 3) Add a constant to $\log_{10}$ of each x value.

3.4.4.2 Take antilog of sum of a constant with each point in a data set.

ANTILOG
Alt A takes the antilog of the current data set

filename *.alg
(Alt 3) Take antilog of sum of constant and each x value.

3.4.4.3 Polynomial transforms

POLY_OPTS
Alt 4
filename *.xfm
The general polynomial transform is a way to combine what might otherwise be several operations. For instance, a data set can be offset and scaled in one operation by setting the first order coefficient to the scale factor and setting the constant term to the offset. Linearization operations that involve higher powers can likewise now be done in one step. In the CD instruments this sort of transformation will allow recorded dynode voltage to be converted to absorbance. Unneeded higher coefficients can be left zero of course.

3.5 Fitting

3.5.1 Linear regression and simple statistics

The programs are able to calculate simple statistics on the points in the current view. The slope is calculated by linear regression. The command **STATS (Alt 2)** gives the following report on the message line:

178 pt, -0.024085 mn, 0.0002 rms, 5.2757E-007 b +/-5.5956, -0.024198 y

The report includes in order: the number of points, the mean of the y values, standard deviation or rms value, the regression coefficient or slope of the data, 5% confidence interval, last y value encountered in view. The confidence intervals are based on normal statistics, not t statistics. The program uses 1.96 * standard error.

3.5.2 Multiple Linear regression

Multiple linear regression is used to calculate the fractions of known library spectra in a test spectra. The test spectra is assumed to be a linear combination of the library spectra. The following equation describes this assumption mathematically

$$Y = A_1 * L_1 + A_2 * L_2 + \ldots + A_0$$

Where Y is the "unknown" test spectra, the "L"s are the library spectra, and the "A"s are the coefficients in the linear combination. A_0 is a constant term.

To select the library spectra ("L"s in equation) to regress against. use **F8** to get the file information on the message line. When the desired spectra are located tag them

using **Alt T**. After selecting the library the test spectra must be located. F1 is used to signal the program to calculate the best fit using the tagged spectra.

The MLR generates the following type of report:

Multiple Linear Regression Results

__n__points	51			
__x__range	190.0 to 240.0 nanometers			
__x__step	1.00 nanometers			
__chi__square	3.9375E+006			
__F__statistic	4540.478			
__correlation__coef	0.9987			
__sum__of__weights	2.52591			
basis set name	basis weight	std. err.	fract. weight	basis fract.
alpha	1.15777	0.058	0.0019	0.45836
beta	0.69438	0.135	0.00114	0.2749
rand	0.54605	0.088	0.0009	0.21618
turn	0.12772	0.074	0.00021	0.05056
__constant__term	-607.14014	976.589	-0.99596	
__source__data__name	bsa			

When you are ready to go on - Strike a Key:

The report summarizes the fitting process: it provides information about the fitted data, gives coefficients ("A"s in equation) as well as a constant term and statistical parameters providing a measure of the goodness of the fit.

A fitted spectra is generated using the coefficients and the library spectra. The fitted is displayed with the extension *.mlr.

3.6 Data synthesis

3.6.1 Lines

$Y = P2 * (X - P1) + P3$

GEN__SET__X__MN x value P1
GEN__SET__Y__MN y value P3
GEN__SET__SLOPE slope of line P2
GEN__STR__LINE needs parm "lin"
uses last value of stats to generate a straight line
*.gen

3.6.2 Gaussians

$Y = P3 * \exp [- \{ P2 * (X - P1)^2 \}]$

GEN_SET_X_MN peak position P1
GEN_SET_Y_MN amplitude of peak P3
GEN_SET_SLOPE 1/bandwidth P2
GEN_STR_LINE needs parm "gsn"
values must be entered in command file

3.6.3 Exponentials

$Y = P3 * \exp [- \{ P2 * (X - P1) \}]$

GEN_SET_X_MN P1 time offset
GEN_SET_Y_MN P3 Amplitude
GEN_SET_SLOPE P2 rate
GEN_STR_LINE needs parm "exp"
values must be entered in command file

3.7 Miscellaneous Data Set Functions

3.7.1 Data Set Overlays

Placing multiple data sets in the current viewing area is a useful feature supported by both the instrument and Plot programs. Two distinct types of data set overlays are possible: **OVERLAY_VIEW (Alt X)** and **OVERLAY_DATA (Alt Z)**. Both overlay types involve selecting a data set from memory and displaying this data set on top of the data set currently graphed on the screen.

OVERLAY_DATA displays the selected data set on top of the current data set using the coordinate system currently on the screen. This results in both data sets being scaled to the same x and y units. If the x-axis range of the second data set is different from the current view, only those points which overlap are shown. If the y-axis of the second data set is greater than the current view, the data is clipped at the boundaries of the current view, and appear as straight lines at either the top or bottom of the graph depending on the values involved. This command assumes that the actual units are the same between the two data sets. If the actual units are different, the magnitudes are used in scaling. This type of overlay is most useful for comparing similar data sets, e.g. the far-UV CD spectra of two proteins.

OVERLAY_VIEW displays the view of the selected data set on the view of the current data set. The actual of the selected data set is superimposed on the current picture. No scaling of data is involved, clipping is as in the view of the selected data set. This type of overlay is useful when comparing data sets which have different y-axis magnitudes and similar x-axis ranges, e.g. dynode voltage vs

wavelength compared to absorbance vs wavelength. This function also allows two similar data sets to be separated in one graphic image.

3.7.2 Data Set Extraction

The current set of points in the view can be extracted into a new data set. This is accomplished by using **EXTRACT (Alt 1)**. This creates a new data set with the name *.ext.

3.7.3 Changing Axis Labels

Alt Y changes the Y axis label
Alt 3 Alt Y changes the X axis label

Section 4 Software Operation of Instrument

4.1 Introduction

The standard method of operating the AVIV instrument is from the keyboard of the system computer. The operator commands the instrument by pressing specific keys which instruct the instrument to perform specific functions. When a function has been invoked, the instrument often asks the operator for additional information. Once the information is supplied the function is performed.

Standard abbreviations in the keyboard system **Ctrl**, **Shift**, **Alt** mean to HOLD DOWN the named shift key and tap the named key following. (i.e. there are 4 cases for some keys). "Toggle" controls alternate between two states (like on/off) and take effect immediately. Commands that take numeric values produce a prompt on the message line. The prompt gives the present value of the associated parameter and asks for a new value. You may enter a new value and press enter to change the value. Simply pressing enter leaves the value unchanged. Typing errors can be corrected by backspacing over mistakes.

4.1.1 Scan and Graph Parameters

Across the top of the screen are 7 lines of text which give information about how the instrument is (or was) set to collect data. This information is stored in the data file as the data set header. The first line is used to display error and alert messages to the operator. The second line has the software version number and ends with system date and time. The third line Starts with the creation date and time. The fourth line begins with scan information and ends with filename. The fifth line starts with the y scaling parameters and ends with motion status or program status. Line 6 is the note line and line 7 is the message/prompt line. The content of most lines can vary depending on the setup of the instrument and will be described in the appropriate section.

4.1.2 Current operating status

Down the left side of the graph is an area that shows the current operating state of the machine. The information here gives hardware settings (wavelength and

slitwidth), instrument operational values (op_level, dynode voltage, CD signal), and code flags. Several other pieces of information are shown in this region: temperature of thermometer, bath setpoint, external channel value, and in kinetics mode the elapsed time. Figure x.y shows many of the code flags and their location. Table x.y lists the code flags and describes what each code represents.

4.2 Adjusting operating controls

4.2.1 Setup Mode

Most of the operating controls can only be changed while in setup. Setup is toggled on by pressing **F6 (MAKE_SETUP)**. When setup is selected it clears the current graph and places the name .setup as the file name. .setup is a special file which cannot be saved, deleted or renamed. No data points are recorded in the file, although the current signal is always plotted on the graph. Some choices to be made when in setup are wavelength settings, the spectral bandwidth, the step size, the mode of data collection and whether to collect auxiliary data sets.

One significant feature of setup is that the scan parameters on the screen at the time you press **F6** are preserved when .setup is created. This allows the use of scan parameters from an existing spectrum to be used as the starting values for a new scan. The scan parameters can be adjusted as needed before scanning begins.

4.2.2 Graph Limits & Recording Limits

The data is presented graphically on the monitor, and the axes of the graph can be shifted and scaled as desired. For data collection the X axis can be in nanometers, seconds, or degrees Centigrade. The Y axis is in millidegrees for CD and either Absorbance or percent transmittance for spectrophotometers. The graph X axis limits set the data collection range. The Y axis limits only apply to graphing the data and do not influence the range of values that are recorded. The actual measured signal is determined by hardware, regardless of whether or not it will fit on the display.

The 4 graph extrema are displayed on lines 4 and 5 of the header. These parameters are updated as the graph limits are changed. The cursor keys are used to adjust the graphing parameters. To use the cursor keys Num Lock should be off (light off), pressing an arrow key will produce a prompt on the message line, giving the operator the option of changing the parameter. The four arrows are well described by their command system names: **RIGHT = SET_RIGHT, LEFT = SET_LEFT, UP = SET_UPPER**, and **DOWN = SET_LOWER.**

4.2.3 Redrawing the Screen

After changing graph parameters the graph is not redrawn until you tell the program to redraw the graph. **HOME (REPLOT)** uses the parameters shown in the data set

header to redraw the graph. **END (FIT_Y)** uses the existing x scale, but adjusts the Y scale to make all of the data visible. **CTRL HOME (FIT_XY)** adjusts both the X and Y scales so all of the data is displayed.

4.2.4 Bandwidth Control and Slitwidth

Spectral bandwidth is maintained constant despite the non-linear dispersion of the monochromator. The "B" flag indicates that the instrument is in constant bandwidth mode. The slit width is adjusted to maintain the bandwidth setting as the wavelength is changed. The current bandwidth is displayed on header line 4. The bandwidth is adjusted by using **F1 (SET_BANDW)**. The spectral bandwidth can be set between 0.01 and 12.00 nm. In the far UV the dispersion of double prism monochromators (60, 118) is very large and the mechanical slits have a maximum opening, such that with some bandwidths the observed resolution is greater than specified.

The auto-bandwidth mode can be turned off with **F5 (TOGL_BANDW)**, but will always be on when during data collection. The slits can be set to any value between 0 and 3 mm. The precision varies with the slitwidth, for 0 to 0.4 mm 4 places are given, between 0.4 and 3 mm 3 places are given. **Alt F5 (GOTO_SLIT)** is used to set the slit width when not in bandwidth mode.

The slitwidth value can be recorded as an auxiliary data set. **TOGL_SLIT_AUX (Ctrl F4)** turns slitwidth tracking off and on. In this mode the "w" flag is shown next to the value of the slitwidth.

4.2.5 Step Size

The size of steps between data points is set using **F3 (SET_STEP)**. This sets the spacing between data points during scanning in wavelength, temperature, and kinetics modes. The step size value is shown on line 4 of the screen header. The scanning procedure is to record a data point, determine where the next point is to be collected, move as quickly as possible to the new location, wait until the new data has settled, record the new point, etc. until the final scan limit is reached.

4.2.6 Averaging Time and Time Constant

It is possible to set the length of time the instrument collects data at each point during a wavelength or temperature scan. This time is called the averaging time. It is shown on line 3 of the screen data header as AvT in units of seconds. This value is set with **SET_TIMC (F7)**. The program works by collecting and averaging data for a short period of time, then checks to see if the AvT time has been exceeded. If the time is not exceeded more data is collected, if the time is complete, the instrument moves to the next point. This averaging of data greatly improves the precision of the data collection beyond that normally associated with Analog to

digital convertors. This feature also prevents any spectral smearing, as might happen when setting the scanning rate in a conventional instrument.

In kinetics mode the signal is damped by a software digital filter. The time constant of this filter is set with **SET_TIMC (F7)**. This is a software damping and should not be confused with the hardware time constant of the instrument.

4.2.7 Temperature of the Sample

The optional thermometer gives a direct reading on the DS screen. All temperatures are given in degrees Celsius. The temperature is shown on the left side of the screen along with the instrument operating parameters (figure). The value of −100.0 is used to signify that the thermometer is not connected. The value of the temperature, when a scan is started, is recorded in the data set header. The creation temperature, CrT, is shown on line X.

4.2.8 Time-Stamping

Each data set is time-stamped upon creation. On screen this information is written on line 3 as "taken -date- at -time- ." The time and date of creation is saved as part of the data set header. The creation date and time can not be modified and is useful in determining when a data set was collected or last modified.

Do not confuse the creation date and time with the current date and time. The current system date and time, including seconds is the constantly changing display at the end of line 2.

4.2.9 Operating level controls

ctrl F5 and ctrl F8
The instrument operating level is controlled by a digital "PID" servomechanism that has a variable setpoint and 3 adjustable parameters. These keys allow you to see the current values of these variables and change them if desired. In general larger values of the gain and derivative constant and smaller values of the integral constant will lead to faster response, but you must be careful not to drive the system into oscillation when adjusting them. You should remember that the system operates over a very large range of dynode voltages. Since the setpoint is saved as part of the data header, the program will not allow you to change the setpoint while a recorded spectrum is on screen.

The Dynode voltage can be recorded as an auxiliary data set. This is useful in the CD to look at a signal that is related to Absorbance. The dynode voltage is recorded in the file "absorb.ads". To start recording Dynode voltage use **TOGL_DYNO_AUX (Alt F8)**.

The op_level can be recorded as an auxiliary data set. To start recording the op_level use **TOGL_OPLV_AUX (Alt F7)**. The op_level is recorded int the file "??.ads".

4.2.10 Starting Data Collection

TOGL_SCAN (Alt F10) toggles data collection on or off in all data collection modes (except Rep_scan, see section ???). **TOGL_SCAN** will start data collection or will abort data collection in progress. When data collection is started a data set recording area, name scan.ads, is created to hold the data. If scan.ads already exists in memory and has not been saved, the program prompts:

scan.ads is not saved. OK to delete? Type y or n

If you choose n, the scan will abort. You should then change the data set name before starting again.

TOGL_SCAN can start data collection from setup or another data file. The data collection parameters from almost any existing data file can be used as the template to control the data collection process.

4.3 Data Collection Modes

The Instrument will collect in several different mode. There are three basic data collection modes of operation: wavelength, kinetics (time), and temperature. These are characterized by the x axis units used to record the data. A fourth mode automates collecting repetitive data. The operation of the instrument in each of these modes is outlined in this section.

4.3.1 Wavelength Mode

Wavelength mode records data over a specified range of wavelengths, at a specified step interval. The data is collected at constant bandwidth. To switch the instrument to wavelength mode (only from setup), use **ENTER_WAVE (Alt W)**. The upper and lower limits default to the current maximum wavelength limits (set in autoexec.avi). The operator must consider several operating parameters before beginning a scan. These parameters can be inherited from an existing data set by creating setup from that file or by starting a scan with the data set on the screen.

The information about the scanning parameters is shown on header line 4.

scan from Ulim.00 nm to Llim.00 nm every Stp.00 nm w/ Bw.00 nm bw

The parameters to be set are as follows:

-Start and End wavelengths - RIGHT and LEFT arrows. They must be between the operating limits specified in the autoexec.avi file (0.01 nm accuracy)
- Wavelength Step-size - F7. It must be between 0.01 and 999.99 nm (0.01 nm accuracy)
- Averaging Time Delay which program can be set with F5. It must be between 0.10 and xx seconds (a tenth of a second accuracy).
- Bandwidth - F1.

To start a wavelength scan use the normal scan toggle Alt F10 or Shift F7 to initiate a repeat.

Wavelength mode works by moving the monochromator to the starting wavelength and slitwidth. The program waits a short time for the instrument to settle. The measurement is performed using the specified averaging time and bandwidth. The point is displayed on the screen. After each point, the program calculates the next wavelength using the step size specified. Wavelength scanning is always from longer to shorter wavelengths, the current wavelength is decremented by the stepsize. Then the program moves the monochromator to the new wavelength and slit position. This is repeated until the end wavelength is reached or exceeded. At that point, the wavelength scan is completed and the monochromator returns to the starting wavelength and slitwidth.

Wavelength scanning is limited by both absolute monochromator limits and user set software limits. The program insists that the starting wavelength is greater than ending wavelength. If the starting wavelength is smaller than the ending wavelength the program switches the values.

File things

Information specific to wavelength scans in the data set is stored on to disk.
All data sets with wavelength on the x axis will have the creation temperature.
If temperature was controlled while the data was collected then a controlled temperature flag is saved with the data in the file. Also, the equilibration time delay is stored with the data if the temperature was controlled. The x axis units are nanometers

When a data set is loaded into memory from disk, the creation temperature is displayed. If the controlled temperature flag is in the data header (the data was recorded in temperature controlled mode) then the equilibration time is also displayed. The temperature setpoint flag is not automatically set until the user sets the setpoint temperature, or creates a setup file from this file, or toggles on a scan while this file is on the screen.

holding = * in 14 pgm

4.3.2 Kinetic Mode

Kinetic mode records data over a specified time, at a specified time interval. The data is collected at constant wavelength and bandwidth. To start kinetics mode (only from setup), use **ENTER_KINET (Alt K)**. The operator must consider several operating parameters. These parameters can be inherited from an existing data set by creating setup from it or by starting a scan with the data set on the screen.

record at xxxx.xx nm for xxxxx.x S, every xxx.x S w/ xx.xx nm bw

The parameters to be set are as follows:

- Wavelength (constant) at which to record data can be set with Alt F6.
- End Time can be set using the RIGHT arrow. (a tenth of a second accuracy) largest time ??
- Time Step-size or interval can be entered using F7. It must be between 0.1 and 999.9 sec (tenth of a second accuracy)
- Time Constant is set with F3. It must be between 0.1 and seconds (a tenth of a second accuracy).
- Bandwidth can be set using F1.

To start a scan in kinetics mode use the normal scan toggle Alt F10 or Shift F7 to initiate a repeat.

less error checking and data validation in kinetics mode

Moving to any wavelength

0.01 precision

You can move the monochromator to any wavelength within the range of the instrument by typing Alt F6 (GOTO_WAVE). The program will prompt

current wavelength 546 goto wavelength:

setting the # of points and time interval

end time update as needed

4.3.3 Temperature Mode

There are several different temperature related operations:

1) Temperature Setpoint Mode
2) Temperature as a Auxiliary Data Set
3) Temperature Mode

4.3.3.1 Temperature Setpoint Mode

In temperature setpoint mode, the operator specifies a setpoint temperature between -30.0 and 100.0 °C. A thermal equilibration time for the sample, can also be specified from 0.1 to 99.9 minutes. This is the time the program waits, after reaching the setpoint, for the sample temperature to stabilize before taking data.

To enter the setpoint temperature, use **SET_TEMP (Shift F1)**. The program will prompt for a new setpoint temperature. If a valid temperature (between -30.0 and 100.0 °C) is entered, it becomes the new setpoint temperature. If no value is entered then the setpoint is unchanged. When temperature control is on, the setpoint temperature appears below the current temperature field (fig VV). As soon as the new setpoint temperature is entered, the program starts to bring the sample to that temperature.

Equilibration

Since the sensor may not be in the sample, there may be a lag between the sense point reaching a new temperature and the sample reaching that temperature. The equilibration time delay starts only after the program has decided that the new temperature has been reached. This delay is intended to allow the sample to reach the final temperature. The time needed may increase as the temperature gets further from ambient.

You can estimate the equilibration time needed by comparing in kinetics mode the response to a small step temperature change near the most extreme temperature with the sensor placed first in the normal sense point and then placed inside a cuvette containing water. (See the thermometer calibration note if you need more information on how to do these experiments.)

Equilibration time is set by Shift F2 key. Because it is kept in the data header it may not be changed after recording. If the value is unspecified or 0, the program will ask for a value whenever a scan is started.

(It is currently difficult to compare up and down staircase data sets because the points are recorded in opposite directions. One of the sets must be reversed off line.

Call us if you want to do this and are having trouble. A future software version will have a function to reverse the order of points built into the program.)

To set the equilibration time delay (while in setup only) use **SET_EQUIL (Shift F2)**. The program prompts for a new time. The operator should enter a numerical value between 0.0 and 99.9 (tenth of a minute accuracy). The equilibration time is displayed in the first line of the screen data header. If a value too small or too large is entered the program uses the closest allowed value.

In temperature setpoint mode, the current sample temperature is controlled at the setpoint value. To enable temperature setpoint mode, use **TOGL_TEMP_MD (Shift F3)**. The temperature setpoint flag, the letter "S", is displayed next to the setpoint value. In addition to displaying the setpoint value, this mode adds a flag to the data set that indicates the temperature was controlled. This flag is indicated by the letters "TMP" in front of the file name.

Temperature can be included as a data validity criterion during wavelength recording. In temperature setpoint mode, the system will not start collecting wavelength scan data unless the current sample temperature is at the setpoint value. If the sample temperature should deviate by more than 1 °C from the setpoint temperature, data collection will stop until the sample temperature returns to the setpoint temperature.

The setpoint temperature and setpoint flag cannot be changed during wavelength data collection (while a scan or a repeat is on). In kinetics mode there is no temperature restriction on data collection, even if the control flag is on. In fact, the setpoint can even be changed during recording, allowing temperature response times to be studied.

Temperature Step Complete Decision Parameters.

There are two independent parts to the decision that the temperature is at a new setpoint, first that the temperature is stable, and second that the temperature is reasonably near the expected value. Each of these parts has several adjustable parameters. These parameters are accessible via function key Ctrl F7. Unlike most of the instrument controls, these values can be changed at any time if necessary. These values are not currently saved in the data set header.

Note that if you constantly use the instrument with a different set of values you can place the commands to set them in your startup command file or in a separate file that you execute as needed.

The operation of the decision process is visible in a status display that appears at the top of the screen when temperature control is turned on. The display looks something like this:

i 1 d 0.050 r 1 s 20.020 a 19.023 e 0.987 t 0.400

The update interval for this display is the first adjustable parameter. (Default interval is .2 minutes.) It is important to note that all rates and time factors in the decision process are expressed in multiples of this interval, not in absolute time.

The temperature is considered stable when the magnitude of the estimated rate of change of temperature is smaller than a specified value for a specified number of time intervals. The criterion for a small rate of change (small first derivative) is the second adjustable parameter. The current derivative estimate (°C per interval) is shown in the status display as the d value (0.050 in the example above).

The minimum number of stable intervals required to decide temperature is stable is 4 time intervals. A longer wait may be necessary to eliminate mistakes at points where the sign of temperature change reverses; this extra number of periods is the third adjustable parameter. The number of periods remaining before the temperature will be considered stable is shown in the status display as the r value. If this number is 0, the temperature is stable. In any time interval where the magnitude of the derivative is found to exceed the size limit, the r counter is reset to its maximum value (4 plus however many extra intervals are selected), otherwise r is decremented until it is 0.

The second criterion for temperature being at a new setpoint is that the temperature be reasonably near the expected value. There are actually two criteria, a loose tolerance used when starting (fourth parameter), and a tight tolerance used once the program has an estimate of the size of the discrepancy between its sensor and the bath (fifth parameter).

The current tolerance in use is shown in the status display as the t value. The best estimate of the temperature which will be reached is shown as the s value, and the actual measured temperature is shown as the a value. (The i value is an internal counter that is only useful to show that time is passing.)

The decision that temperature is in tolerance is based on a comparison of a smoothed estimate (e) of the error between actual (a) and expected (s) temperatures to the current tolerance (t). The rate constant used in
generating the smoothed error estimate is the sixth choice in the list of parameters. A value of 1 for this rate constant means that error terms from previous intervals are ignored, smaller values produce more smoothing, a longer memory for past errors, and more of a lag in the error settling below the tolerance limit.

The initial value for the expected temperature (s) is the first setpoint. The decision that temperature is stable at this first point is made using the loose tolerance. For the second point the program updates s by the step size and adds the error term for

the difference between the asked for set point and the actual temperature reached. Because of this adjustment, the expected value for the second point should be much closer to the actual value reached at the second point. Therefore the program switches to the tight tolerance for the second and subsequent points.

At each later temperature step the estimate of the next temperature to be reached (s) is updated by the step size and by a correction factor derived from the smoothed temperature error estimate (e). This update allows the tight tolerance to be kept small by compensating for drift in the analog temperature signals, for non-linearities in the temperature measurements, and for change in the difference between bath and sense point temperature due to change in the rate of heat loss. The weighting factor for the amount of the current error to add to the next temperature estimate is the last parameter.

Note that the steps sent to the bath are not affected by this process. Closed loop control of temperature is possible but is slower. If the bath is well coupled to a well insulated cell holder then performance will be quite good with this open loop system.

4.3.3.2 Temperature Auxiliary Data Set

The program can record temperature as an auxiliary data set, each point corresponding to a data point in the main data set. To toggle on or off recording an auxiliary temperature data set use **TOGL_TEMP_AUX (Shift F4)**. A "T" flag will appear at the left edge of the screen by the actual temperature display to indicate that an auxiliary data set (s_temp.ads) will be created when a scan is started. This flag can not be toggled on or off during data collection. Also, the temperature does not have to be controlled to record an auxiliary temperature data set.

In kinetics mode the auxiliary data sets are not buffered the way the main data set is. If collection is interrupted by some operation, (e.g. loading a file), the main data points will be correct in time, but the auxiliary data points may not be. The auxiliary data points are taken only after the main data points are copied out of the holding buffer.

4.3.3.3 Temperature Mode

Temperature mode records CD values over a specified range of temperature, at a specified resolution interval. The data is collected at constant specified wavelength and bandwidth. To start temperature mode (only from setup), use **ENTER_TEMP** (Alt T). Temperature mode turns on temperature control if the setpoint flag was not on. The setpoint temperature and upper and lower limits default to the current temperature if the setpoint flag was not on (the step size defaults to 0.1 °C). If there was a setpoint temperature, it is left unchanged and the limits are set to it. The

operator must set consider several operating parameters. These parameters can be inherited from an existing data set by creating setup from it or by starting a scan with the data set on the screen.

at xxxx.xx nm go from xxx.x C to -30.0 C by -20.x C w/ xx.xx nm bw

The parameters to be set are as follows:

-Start and End Temperatures can be set using the RIGHT and LEFT arrows. They must be between -30.0 and 100.0 °C (a tenth of a degree accuracy)
- Temperature Step-size or interval can be entered using F7. It must be between 0.1 and 99.9 °C (tenth of a degree accuracy)
- Equilibration Time Delay which program is to wait after reaching a temperature can be set with Shift F2. It must be between 0.0 and 99.9 minutes (a tenth of a minute accuracy).
- Wavelength (constant) at which to do the melt can be set with Alt F6.
- Bandwidth at which to do melt can be set using F1.

To toggle on the simple staircase use the normal scan toggle Alt F10 or Shift F7 to initiate a repeat.

Temperature mode works by setting the setpoint temperature to the starting temperature and waiting for the temperature control system to bring the sample to that temperature. It waits the equilibration time delay specified by the operator before measuring the CD value at each temperature. The CD measurement is performed using the specified averaging time and displayed on the screen. After each point, the program calculates the next temperature using the step size (interval) specified by the user. The program knows, from the start and end temperatures, which direction the staircase will go. That is, whether to decrement or increment the temperature by the stepsize to calculate the next temperature. Then, it brings the sample to the new temperature and waits the equilibration time again before measuring the next point. This is repeated until the end temperature is reached or exceeded. At that point, the staircase scan is completed. The setpoint temperature is left at the final temperature.

Temperature parameters stored to disk:

When the data set is stored on to disk, other information is stored with the data in the file in a data header preceding the data values. All data sets with time or wavelength on the x axis will have the current temperature at the beginning of the scan as the creation temperature. A temperature staircase data set has start and end temperatures but does not have a creation temperature. The creation temperature is stored with the data in file. If temperature was controlled while the data was collected then a controlled temperature flag is saved with the data in the file. Also, the equilibration time delay is stored with the data if the temperature was controlled.

The x axis units are stored with the data to indicate whether this data was recorded in wavelength, temperature, or time mode. Other data related information such as data set name, some scan parameters, creation date and time, and the y axis units are stored for every data set.

When a data set is loaded into memory from disk, the creation temperature is displayed, except for a staircase data set which does not have a creation temperature. If the controlled temperature flag is in the data header (the data was recorded in temperature controlled mode) then the equilibration time is also displayed. The temperature setpoint flag is not automatically set until the user sets the setpoint temperature, or creates a setup file from this file, or toggles on a scan while this file is on the screen.

Inheritance:

If the user creates a setup data set or starts a scan, and the current data set was created with temperature controlled then the new data set inherits temperature control. The creation temperature (or starting temperature in the case of a staircase data set) of the data set on the screen is inherited as the new setpoint temperature for the new data set. If the screen is a blank data set, when the x axis is switched to temperature, then the setpoint temperature is set to the current temperature. The equilibration time of the current data set is also inherited by the setup data set. The equilibration time of the setup data set will be used if a scan is initiated while setup is on the screen. If the parent data set was not temperature controlled, then if temperature setpoint was on, it is turned off. Note that the temperature setpoint flag stays the same even if setup mode is turned off until some other event changes it.

4.3.4 Repetitive Scanning

The Repetitive Scanning (Rep-Scan) allows the user to automatically collect a series of scans of the same sample and average them improve the signal to noise ratio.

4.3.4.1 How Repetitive Scan works

Rep-Scan collects data sets and shows the data as it is collected on the screen. When each scan is complete, the data set is added to an accumulator data set (accum). The accumulator is then divided by the number of scans completed, resulting in the average (rep_avg). The delay time is the time interval between starting one scan and the time of starting the next scan. If the time delay runs out before a scan is finished, then the next scan starts as soon as the current is done. If there is time between scans the average is shown, otherwise the next scan is started. Unless stopped, Rep-Scan will repeat this process the number of scans specified. While a scan is being collected (or between repeats), the user can look at the average or the accumulator as well as other data-sets. The user may choose to keep all data sets created during Rep_scan. The successive scans are kept under a user supplied name

with an extension (.001, .002, etc.) indicating the position of the scan in the sequence.

The setup file (.setup), the accumulator (accum), the average (rep_avg), and the current scan data set are protected from being renamed or deleted during Rep_scan.

4.3.4.2 How to set up for a Rep-Scan run

In setup mode the user can set the number of repeats and the minimum time delay between scans, as well as set the scan parameters. When toggling setup, if the current data set was collected in Rep_scan mode then .setup will inherit the number of repeats and time delay from that file. .setup becomes the template used for scanning in Rep-Scan.

Shift F6 () sets the number of scans to be collected. The program will prompt

repeats default value: new value:

the user can then enter a value between 1 and 9999. Shift F5 sets a delay time between scans. The program will prompt:

display the current (or default) delay in minutes and ask you to

the user can then enter a new value between 0 and 59 minutes.
If you hit <return> without entering a number or enter an invalid number (eg. a negative number or a letter), the program keeps the current value.

To save all scans set the parameter to one when asked about saving scans, in **Shift F5**. All intermediate scans will be saved using a name supplied by user as *.001, *.002, etc.

4.3.4.3 How to operate Rep-Scan

Rep-Scan is toggled on by Shift F7 (). Rep-Scan can not be turned on if there is another scan in progress. When Rep-scan is on, the R flag appears (), and will stay on until Rep-Scan is turned off.

Rep-Scan is toggled off by Shift_F7 (). If Rep-Scan is in the middle of a scan (collecting data) when it is turned off, rep-scan will make this scan its last repeat regardless of the number of repeats to be done. Rep-scan will continue this scan to the end and then use it in calculating the average before displaying the average. When Rep-Scan is off the user can toggle the scan off with Alt F10. In this case the last scan is not included in the average.

When the last scan is completed in rep-scan, the final average will be displayed. If the user toggles off both Rep-scan and the scan, while the scan is in progress, the

unfinished scan will be displayed. If the scan is not the first repeat, the average will be available in the ring (memory). The accumulator is deleted when Rep-Scan is done.

Section 5 The Command System

The following pages provide a more detailed description of the extended command and log system. We discuss the exact form of commands and some of the special requirements which arise when executing a list of stored commands. We also describe some new commands in the extended system which are not accessible at present directly from the keyboard. The end of this document provides several lists of the commands sorted in different ways.

5.1 Introduction to extended command system

The command system was created with a dual purpose. Command files allow easy customization of the instrument and allow commonly used function sequences to be grouped in a single operation. Command files also allow the instrument to be controlled from another computer by having the instrument execute COM1, the serial port. Logs are also dual purpose, they allow recording of the instruments operation locally, and they provide a way for the instrument to report back to a controlling computer if a log is opened to COM1.

5.1.1 Command Files

A command file is a series of commands, as defined below in detail. Command files can be stored on the disk or they can be received from the serial port. Several command files can be open at once. Execution of command files is nested. Commands are read from a file one at a time and are executed. When a command is completed the instrument looks for the next command and continues in this way until the end of the file is reached. When a command file is exhausted, it is closed. When all command files are closed, control returns to the keyboard.

The first thing the program does on startup is to open and execute an autoexec file, the operator only gains control of the instrument when this file completes. Command file execution can be started from the keyboard with the Alt F1 key. Execution of a nested command file is started from within a command file with the EXECUTE command.

5.1.2 Log Files

When a log file is opened, every function executed by the program is echoed to that log. This can provide a trail of operations for reliability and recovery purposes. A log is also potentially useful for understanding what is wrong if the instrument doesn't act as expected. For this reason, when the instrument is delivered, the startup file is set to open a log called "operate.log" in the "log" subdirectory of the instrument directory. A log can be opened at any time. Use of logs is nested, that is, entries are only made in the most recently opened log. There are actually 2 ways of opening a log, APPEND_LOG and OPEN_LOG. The difference is that open erases an old file if it exists and append does not. Both methods create the log if it does not exist and both write new entries at the end of the file.

5.1.3 Remote Operation

A log file also allows a remote computer to synchronize itself with the operation of the instrument. As each command read from the current command file is completed it is echoed back to the log along with a positive or negative acknowledgement, /*a*/ or /*n*/ respectively. The remote computer can use the ack or nak to pace the sending of new commands. In this way the remote computer is not obliged to use SYNC's.

A function called DATA_LOG_ON causes the program to make an entry in the current log for each data point recorded. This allows the remote computer to monitor the instrument's operation in real time. Because the remote computer does not have to execute SYNC commands, it can stop data recording whenever it decides that enough points have been acquired.

5.2 Language Format

Presently the language includes only commands. The language is free form, not line oriented. All white space is ignored. The definition of white space includes tabs, new lines, and blanks. Space can be used freely to improve the readability of the file. The files are saved in ordinary ASCII.

5.2.1 Commands

Each command has a start character, [, and a terminating character,]. Command names are all UPPERCASE. If an argument is supplied, it is separated from the command name with a comma. Arguments are either numbers or literal text strings, as appropriate. Text strings are always enclosed in quotes, "like this". There can be no more than one argument to a command.

5.2.2 Comments

Anything within "/*" and "*/" delimiters is considered a comment and is replaced by a blank space. Here are some sample command sequences:

```
[ OPEN_LOG , "prn" ] /* the log will go to the printer */
[ MESSAGE , /* the operator sees this message */
   "Ready to log to printer - strike a key" ]
[ SYNC_RESP ] /* wait for the operator to respond */

/* this example causes a 300 second pause */
[TIME_START,300] [SYNC_TIME]
```

In the Appendix the Command names are listed twice. The first list includes only functions accessible from the keyboard. This list is organized by key to make it easy to find commands equivalent to known keyboard functions. The second list is organized alphabetically by command name. The lists include argument type used if any.

5.3 Special Language features

5.3.1 Synchronization

Synchronization commands (SYNC's) are needed whenever the next command in a file should not be executed until a previously started operation, such as a scan, has completed. For example, you cannot rename a data file while data is being added to it. If a RENAME command is executed during a scan the program rejects it. When you run the instrument you know enough to wait, but the command execution program must be told when to pause in reading a command file.

Here is a list of Sync's and the conditions they wait for:

[SYNC_ENTR] - wait for the enter key to be struck
[SYNC_MOVE] - wait for motor movement to stop
[SYNC_PLOT] - wait for plotting to stop
[SYNC_RESP] - wait for any keystroke
[SYNC_REP] - wait for repeat mode collection to finish
[SYNC_SCAN] - wait for data collection to finish
[SYNC_TEMP] - wait for set temperature to be established
[SYNC_TIME] - wait for timer to run out (see TIME_START)

5.3.2 Syntax Checking

When a command file is executed syntax errors will be reported as they are found by the line and column position in the source file. You can abort the execution of a command file after a syntax error is detected or you can continue execution. If the command [SYNTAX_ON] is executed in a file then further command execution

is suppressed, but the scan of the file continues. You can insert this command temporarily in a new command file to check for syntax errors before starting the instrument on a long experiment.

5.3.3 Limited Use Keys

These keys are not functional from a command file, they are included for completeness in logging keyboard operations. Most of these keys offer the operator a fixed series of choices. Each of these choices is given a separate extended function code for use in command files.

```
HELP        A_H      - displays the Help file, keys.lst
DIRECTORY   S_09     - shows disk directory listings
REPT_OPTS   S_05     - repeat mode options
POLY_OPTS   A_n4     - polynomial transform coefficients
SMOO_OPTS   A_n7     - polynomial smoothing choices
PEAK_OPTS   A_n8     - peak picking choices
DYNO_OPTS   C_02     - dynode mode (maintenance feature)
DY_SV_OPTS  C_06     - dynode servo tuning (maintenance)
TEMP_OPTS   C_07     - temperature stability parameters
DEMOD_OPTS  C_PGDN   - spectrophotometer data validation
TM_SV_OPTS  C_RIGHT  - closed loop temperature control
```

5.4 Summary of Commands

Printer Commands

```
FORM_FEED     - sends printer paper to top of next sheet
LINE_FEED     - prints last log line in printer buffer
PAGE_LENGTH   - sets page length used by PRINT_FILE
PRINT_FILE    - print file as it would be saved on disk
PRINT_SCREEN  - performs a screen dump
```

Commands useful with SYNC's

```
KBD_CLEAR     - empty keyboard buffer to prevent typeahead
TIME_START    - starts a timer tested by SYNC_TIME
```

Logging Commands

```
LOG_NOTE        - copies itself to the log for record keeping
LOG_DATA_NAME   - puts name of data set on screen into the log
LOG_TIMESTAMP   - puts the current date and time into the log
STATS           - log descriptive statistics of current screen
```

Remote Operation Commands

SAVE_TO_COM1 - current data to COM1 instead of to disk
DATA_LOG_ON - all subsequent data points are logged
DATA_LOG_OFF - resets data logging mode

Operator Message Commands

MESSAGE - places a message on the prompt line
MESSAGE_CLR - erases the prompt line

Commands to set File Access Paths

PATH_LOG - default path for opening log files
PATH_HELP - path for finding the help file, keys.lst
PATH_DATA - default path for loading and saving data
PATH_COMD - default path for opening execute files

Execution Control

EXECUTE - begin interpreting a new execute file
EXECUTE_STOP - close the current execute file
SYNTAX_ON - suppres interpretation, continue scanning
SYNTAX_OFF - resume normal interpretation

Log Control

OPEN_LOG - open a nested log file, erase any old
APPEND_LOG - open a nested log file, do not erase old
CLOSE_LOG - close the current log file

5.5 Commands Listed Alphabetically

Key to Argument Types

-	- no argument
s	- text, but only up to the first whitespace
c	- confirmation (y, Y, n, or N)
t	- a line of text including spaces
r	- a real number (double prec., frac or exp format)
i	- a signed 16 bit integer
l	- a signed 32 bit integer

Key to program compatibility

U	- Key valid in all programs
I	- Instrument only
P	- key only valid in plot
S	- 14 and 118 only
C	- 60 series CD only
H	- 60HDS only
-H	- all Inst. but 60hds

function name	key	arg	Pgms
ADD	Alt P	U	s
ANTILOG	Alt A	U	r
APPEND_LOG		U	s
AUX_BIT_CLR		I	i
AUX_BIT_COMP		I	i
AUX_BIT_SET		I	i
BASELINE	Alt B	U	-
BTH_DER_TOL		-H	r
BTH_ERR_TIMC		-H	r
BTH_LOOS_TOL		-H	r
BTH_SPL_INT		-H	r
BTH_STL_CNT		-H	i
BTH_TITE_TOL		-H	r
BTH_TRACK_GN		-H	r
CD_CAL_FACTOR		C	r
CD_FILTER		C	i
CD_GAIN_2		C	r
CD_READSPER		C	i
CLOSE_LOG		U	-
CORRECT	Alt C	U	-
DATA_LOG_OFF		U	-
DATA_LOG_ON		U	-
DB_DK_REF		S	r
DB_IDL_SET		S	i
DB_WI_TOL		S	i
DEMOD_OPTS	Ctrl PGDN	I	-
DIRECTORY	Shift F9	U	-
DIVIDE	Alt 5	U	r
DO_POLY_TR		U	-
DYDY_SV_DTIM		I	r
DYDY_SV_GAIN		I	r
DYDY_SV_ITIM		I	r
DYDY_SV_SPT		I	r
DYNODE_MD		I	i
DYNO_OPTS	Ctrl F2	I	-
DY_SV_DTIM		I	r
DY_SV_GAIN		I	r
DY_SV_ITIM		I	r
DY_SV_OPTS	Ctrl F6	I	-
ENTER_KINET	Alt K	I	-
ENTER_TEMP	Alt T	I	-
ENTER_WAVE	Alt W	I	-
EXECUTE	Alt F1	U	s
EXECUTE_STOP		U	-
EXTRACT	Alt 1	U	-
FIT_XY	Ctrl HOME	U	-
FIT_Y	END	U	-
FLIP	Alt F	U	-
FORM_FEED		U	-
GEN_SET_SLOPE		U	r
GEN_SET_X_MN		U	r
GEN_SET_Y_MN		U	r
GEN_STR_LINE		U	s
GOTO_SLIT	Alt F5	I	r
GOTO_WAVE	Alt F6	I	r
HELP	Alt H	U	-
HOME_ALL	Alt F4	U	c
HP_OVSH_TEMP		H	r
HP_OVSH_TIME		H	r
HP_PROB_CTL		H	s
HP_REINIT		H	c
HP_STIR_CTL		H	i
HP_TEMP_SRC		H	s
HP_UNIT_SEL		H	s
INVERSE	Alt V	U	r
IR_ENAB		S	i
KBD_CLEAR		U	-
LINE_FEED		U	-
LOAD_FILE	Alt L	U	s
LOG	Alt U	U	r
LOG_DATA_NAME		U	-
LOG_NOTE		U	t
LOG_TIMESTAMP		U	-
MAKE_SETUP	F6	I	-
MESSAGE		U	t
MESSAGE_CLR		U	-
ML_REGRESS		U	-
MULTIPLY	Alt M	U	r
NAME_OPS	F8	U	-
NEXT	PGUP	U	-
NOTE	Alt N	U	t
NOTE_FULL	Alt DASH	U	t
OFFSET	Alt O	U	r
OPEN_LOG		U	s

OVERLAY__DATA	Alt Z	U	s	SET__EQUIL	Shift F2	I	r
OVERLAY__VIEW	Alt X	U	s	SET__ETST__MD		I	-
PAGE__LENGTH		U	i	SET__EXTN__AUX		I	i
PATH__COMD		U	s	SET__FSR__MD		C	i
PATH__DATA	Shift F8	U	s	SET__FULL__SCR		U	i
PATH__HELP		U	s	SET__LEFT	LEFT	U	r
PATH__LOG		U	s	SET__LOWER	DOWN	U	r
PEAK__DERIV		U	i	SET__OFST__MD		I	i
PEAK__DISCRD		U	i	SET__OPLV__AUX		I	i
PEAK__GLBL__THR		U	r	SET__OP__OFFSET		C	r
PEAK__INTERPOL		U	i	SET__OP__SCALE		C	r
PEAK__LOCL__THR		U	r	SET__OVLY__TAG		U	i
PEAK__OPTS	Alt 8	U	-	SET__PLOT__TAG		U	i
PEAK__PICK	Alt J	U	-	SET__REGR__TAG		U	i
PEAK__S__DERV		U	i	SET__REP		I	i
PEAK__S__DISCRD		U	i	SET__REPS	Shift F6	I	i
PEAK__S__WN__HSZ		U	i	SET__RIGHT	RIGHT	U	r
PEAK__TST__CTL		U	i	SET__SCAN		I	i
PEAK__WN__HSIZ		U	i	SET__SLIT__AUX		I	i
PLOT__ABORT	Ctrl F2	P	-	SET__SLIT__MD		I	i
PLOT__DATA	Ctrl F3	P	s	SET__STEP	F3	I	r
PLOT__FILE		P	s	SET__TEMP	Shift F1	I	r
PLOT__NXT__PEN	Ctrl F8	P	i	SET__TEMP__AUX		I	i
PLOT__PAGE__FD	Ctrl F7	P	-	SET__TEMP__MD		I	i
PLOT__PENS	Ctrl F5	P	i	SET__TIMC	F7	I	r
PLOT__PORT		P	i	SET__UPPER	UP	U	r
PLOT__SCREEN	Crtl F1	P	i	SET__XLINK__MD		U	i
PLOT__TYPE		P	i	SET__X__NEXT		U	i
PLOT__VIEW	Ctrl F4	P	s	SET__ZERO__MD		U	i
POLY__CF0		U	r	SHOW__DATA	Alt G	U	s
POLY__CF1		U	r	SMOOTH	Alt I	U	-
POLY__CF2		U	r	SMOO__DERIV		U	i
POLY__CF3		U	r	SMOO__OPTS	Alt 7	U	-
POLY__CF4		U	r	SMOO__ORDER		U	i
POLY__OPTS	Alt 4	U	-	SMOO__TST__CTL		U	i
PRINT__FILE	Ctrl LEFT	U	-	SMOO__WHSIZ		U	i
PRINT__SCREEN		U	-	STATS	Alt 2	U	-
PRIOR	PGDN	U	-	SUBTRACT	Alt Q	U	s
QUIT	Ctrl D	U	c	SYNC__ENTR		U	-
RATIO	Alt 6	U	s	SYNC__MOVE		I	-
REMOVE	Alt D	U	c	SYNC__PLOT		P	-
RENAME	Alt R	U	s	SYNC__REP		I	-
REPAINT	Alt F2	U	-	SYNC__RESP		U	-
REPLOT	HOME	U	-	SYNC__SCAN		I	-
REPT__OPTS	Shift F5	I	-	SYNC__TEMP		I	-
REP__INTERVAL		I	r	SYNC__TIME		I	-
REP__KEEPNAME		I	s	SYNTAX__OFF		U	-
REP__KEEP__CTL		I	i	SYNTAX__ON		U	-
SAVE__FILE	Alt S	U	c	TEMP__OPTS	Ctrl F7	I	-
SAVE__TO__COM1		U	-	TIME__START		I	i
SERVO__SET	Ctrl F5	I	r	TM__SV__CTRL		-H	c
SET__ALL__PTS		U	i	TM__SV__DTIM		-H	r
SET__ANG__LD		U	i	TM__SV__GAIN		-H	r
SET__AU__MD		I	i	TM__SV__ITIM		-H	r
SET__BANDW	F1	I	r	TM__SV__OPTS	Ctrl RIGHT	-H	-
SET__BW__MD		I	-	TOGL__ALL__PTS	Alt 9	U	-
SET__DYNO__AUX		I	i	TOGL__ANG__LD	Alt F3	U	-

TOGL__ASK__PEN	Ctrl F6	P	-
TOGL__AU__MD	F2	S	-
TOGL__BW__MD	F5	I	-
TOGL__DET	Crtl F10	S	c
TOGL__DYNO__AUX	Alt F8	I	c
TOGL__ER__FLGS	Ctrl PGUP	S	-
TOGL__ETST__MD	Alt F9	I	-
TOGL__EXTN__AUX	Shift F10	I	c
TOGL__FSR__MD		C	-
TOGL__FULL__SCR	Alt EQUAL	U	-
TOGL__OFST__MD	F4	I	-
TOGL__OPLV__AUX	Alt F7	I	c
TOGL__REP	Shift F7	I	c
TOGL__SCAN	Alt F10	I	c
TOGL__SLIT__AUX	Ctrl F4	I	c
TOGL__SRC	Ctrl F9	S	c
TOGL__TEMP__AUX	Shift F4	I	c
TOGL__TEMP__MD	Shift F3	I	-
TOGL__XLINK__MD	Ctrl END	U	-
TOGL__X__NEXT	Alt 3	U	-
TOGL__ZERO__MD	Alt 0	U	-
WAVE__CAL	Ctrl F1	I	l
WAVE__LLIM		I	r
WAVE__ULIM		I	r
WEIGHT	Alt E	U	s
XOV__DET	F10	S	r
XOV__SRC	F9	S	r
Y__LABEL	Alt Y	U	s
Z__OFFSET	Ctrl F3	I	r

5.6 Commands Listed by Keyboard code

Key	Function	arg
Alt F1	EXECUTE	s
Alt F2	REPAINT	-
Alt F3	TOGL_ANG_LD	-
Alt F4	HOME_ALL	c
Alt F5	GOTO_SLIT	r
Alt F6	GOTO_WAVE	r
Alt F7	TOGL_OPLV_AUX	c
Alt F8	TOGL_DYNO_AUX	c
Alt F9	TOGL_ETST_MD	-
Alt F10	TOGL_SCAN	c
Alt A	ANTILOG	r
Alt B	BASELINE	-
Alt C	CORRECT	-
Alt D	REMOVE	c
Alt E	WEIGHT	s
Alt F	FLIP	-
Alt G	SHOW_DATA	s
Alt H	HELP	-
Alt I	SMOOTH	-
Alt J	PEAK_PICK	-
Alt K	ENTER_KINET	-
Alt L	LOAD_FILE	s
Alt M	MULTIPLY	r
Alt N	NOTE	t
Alt O	OFFSET	r
Alt P	ADD	s
Alt Q	SUBTRACT	s
Alt R	RENAME	s
Alt S	SAVE_FILE	c
Alt T	ENTER_TEMP	-
Alt U	LOG	r
Alt V	INVERSE	r
Alt W	ENTER_WAVE	-
Alt X	OVERLAY_VIEW	s
Alt Y	Y_LABEL	s
Alt Z	OVERLAY_DATA	s
Alt 1	EXTRACT	-
Alt 2	STATS	-
Alt 3	TOGL_X_NEXT	-
Alt 4	POLY_OPTS	-
Alt 5	DIVIDE	r
Alt 6	RATIO	s
Alt 7	SMOO_OPTS	-
Alt 8	PEAK_OPTS	-
Alt 9	TOGL_ALL_PTS	-
Alt 0	TOGL_ZERO_MD	-
Alt DASH	NOTE_FULL	t
Alt EQUAL	TOGL_FULL_SCR	-

Key	Function	arg
Ctrl F1	WAVE_CAL	l
Ctrl F2	DYNO_OPTS	-
Ctrl F3	unused	-
Ctrl F4	TOGL_SLIT_AUX	c
Ctrl F5	SERVO_SET	r
Ctrl F6	DY_SV_OPTS	-
Ctrl F7	TEMP_OPTS	-
Ctrl F8		-
Ctrl F9		-
Ctrl F10		-
Ctrl D	QUIT	c
Ctrl END	TOGL_XLINK_MD	-
Ctrl HOME	FIT_XY	-
Ctrl LEFT	PRINT_FILE	-
Ctrl PGDN	DEMOD_OPTS	-
Ctrl PGUP	TOGL_ER_FLGS	-
Ctrl RIGHT	TM_SV_OPTS	-
F1	SET_BANDW	r
F2	TOGL_AU_MD	-
F3	SET_STEP	r
F4	TOGL_OFST_MD	-
F5	TOGL_BW_MD	-
F6	MAKE_SETUP	-
F7	SET_TIMC	r
F8	NAME_OPTS	
F9		-
F10		-
Shift F1	SET_TEMP	r
Shift F2	SET_EQUIL	r
Shift F3	TOGL_TEMP_MD	-
Shift F4	TOGL_TEMP_AUX	c
Shift F5	REPT_OPTS	-
Shift F6	SET_REPS	i
Shift F7	TOGL_REP	c
Shift F8	DEFAULT_DRIVE	s
Shift F9	DIRECTORY	-
Shift F10	TOGL_EXTN_AUX	c
DOWN	SET_LOWER	r
END	FIT_Y	-
HOME	REPLOT	-
LEFT	SET_LEFT	r
PGDN	PRIOR	-
PGUP	NEXT	-
RIGHT	SET_RIGHT	r
UP	SET_UPPER	r