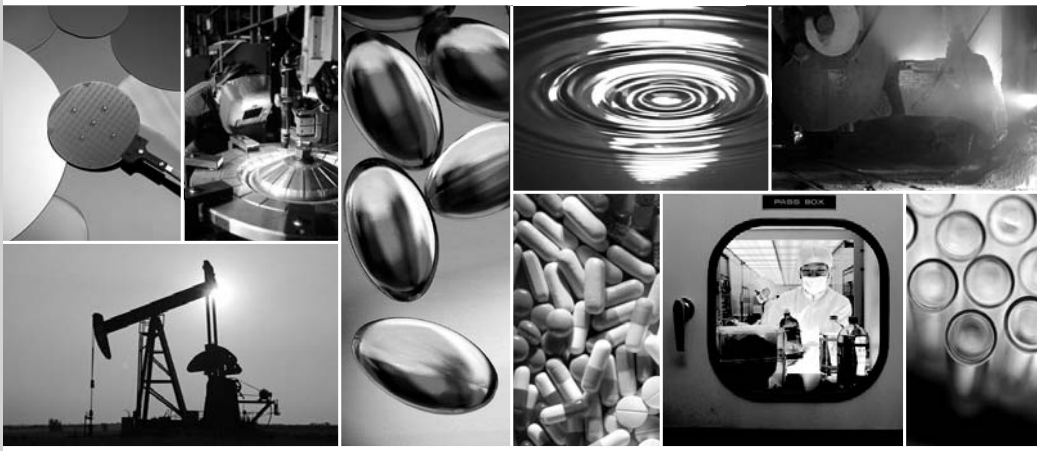
Evolution 500 Local Control Software Manual



Note

This manual is being revised, so some of the information you will find in it is out-of-date. Please accept our apologies for any confusion this may cause. Any reference to Unicam, Spectronic Instruments or Thermo Spectronic has changed to Thermo Electron Corporation, and the contact and trademark information has also changed. On the next page, you will find a current disclaimer and up-to-date contact and trademark information. Please contact Thermo Electron if you have any questions or concerns.

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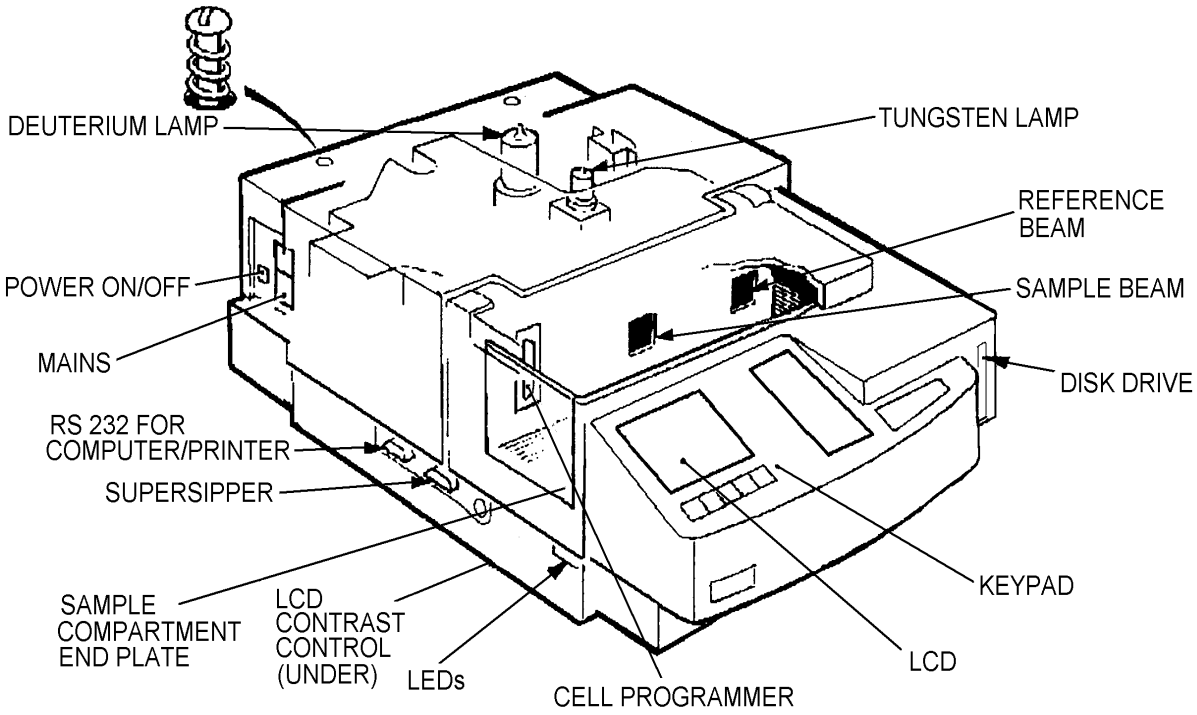
GENERAL

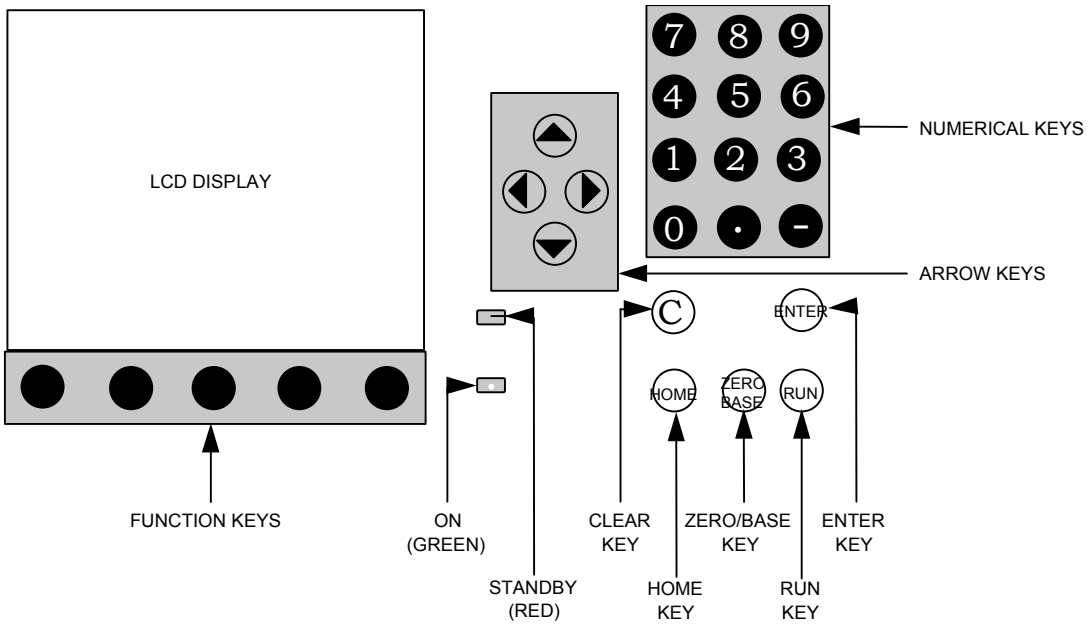
Introduction

- The Nicolet Evolution 500 UV-Visible spectrophotometer can be controlled independently via an integral keypad and LCD display, or externally from a computer. The Evolution 500 is available in both local control and blind bench variants.
- This manual describes the operation of the Local Control software on the Evolution 500 spectrophotometers.
- The system is composed of a spectrophotometer with integral keypad, LCD display, 1.44 Mbyte Disk Drive, Local Control Software and output device.
- Always remove disks from the disk drive when not in use. Never power-up the instrument with a disk in place, as permanent damage may be caused to the disk.[1]
- The Local Control software controls all aspects of the systems operation.
- The UVCalc software accessory is included as standard and provides automatic calculation of results from measurements, using user-defined equations. UVCalc can be used in the SCAN, FIXED and QUANT modes.



[1] The only exception to this rule is when upgrading the instrument software. Then, automatic recognition of a software disk causes an automatic upgrade of the software.

User Interface



Key	Operation
Arrow Keys	Highlight menu options, or move track cursor, or move Cell Programmer, depending on page in use. Change display contrast with <> from Home Page.
Numerical Keys	Enter numbers, minus and decimal point.
Function Keys	Access and perform system functions. Operation depends on screen in use, and is indicated by labels at bottom of screen.
Clear	Clears entry leaving field or parameter ready for new entry, clears pop-up, and clears error messages.
Enter	Enters changes to field or parameter.
Run	Starts instrument measurement according to current method.
Home	Returns to Home page.
Zero/Base	Performs a zero or baseline as appropriate to application.
Indicator LEDs	Lower (green) = ON, upper (red) = STANDBY

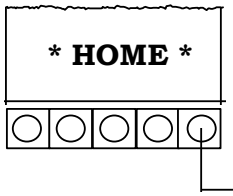
REMOVE THE SAMPLE AND ENSURE THAT BOTH SAMPLE AND REFERENCE BEAMS ARE CLEAR OR CONTAIN THE BASELINE SAMPLES RELEVANT TO THE ANALYSIS BEFORE ZEROING THE INSTRUMENT OR PERFORMING A BASELINE SCAN.

Software

The Local Control Software is organised in a tree structure with all functions accessed initially from the HOME Page. Movement between the software pages is controlled by function keys or by highlighting with cursor keys and pressing ENTER. Home will always go to the HOME page.

The SCAN, FIXED, QUANT, RATE and MCA applications are entirely separate. Only one application can be operational at any one time. Loading another application will overwrite any current data.

Local and Computer Control



- From switch-on the instrument will automatically be under the control of the LOCAL CONTROL software. To enable control from an external computer press REMOTE on the HOME page. Control will go to the computer providing the instrument is idle.

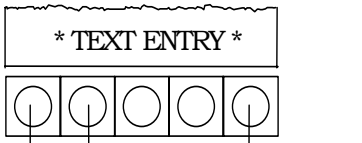
- To return control to the Local Control software press the HOME key. Control will revert to the Local Control software providing that the instrument is idle, and the PC software has relinquished control.

TEXT ENTRY Page

This page is used for entry of method, operator, and sample identities in all applications and for entry of concentration units in QUANT and FIXED methods. The title displayed at the top of the page depends on which parameter is being edited. On entry to this page the name field is filled with the current value.

OPERATOR	Enter up to 11 characters for operator ID.
METHOD ID	Enter up to 11 characters for method description.
UNITS	Enter up to 11 characters for Conc units.
SAMPLE ID	Enter up to 11 characters for sample ID

- Use the Arrow keys to move the cursor to the required character and press ENTER. Once all the required characters have been entered press ACCEPT. Numbers are entered using the numeric keypad. If you make a mistake  will act as a backspace or CLEAR will clear the whole entry.



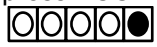
(←) - Acts as backspace and clears the last character in the line.

ACCEPT - Enters the names and returns to the calling screen.

CANCEL - Abandons the naming operation and returns the calling page. The original entry is not changed.

SAVE/RENAME

This page is used for saving or renaming files from any part of the LOCAL CONTROL software. The page is used to name a file and/or change the ID.

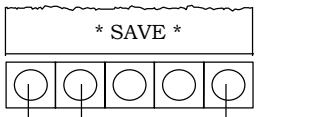
- On coming to the page the Filename field is ready for editing. Use the Arrow keys to move the cursor to the required character and press ENTER. Once all the required characters have been entered press ACCEPT. Numbers are entered using the numeric keypad. If you make a mistake  will act as a backspace or CLEAR will clear the whole entry.

Filenames are limited to 8 characters.

- To change the FILE TYPE highlight the field and press ENTER to display the pop-up menu. Available formats are NORMAL (the native file type of the Local Control Software), CSV (Comma separated variable) and JCAMP-DX (JCAMP data exchange format). Highlight your choice and press ENTER to select.

- The ID field will contain the characters entered for the method. To edit the ID highlight the ID field and press ENTER, change as necessary then press ACCEPT.

- To select the destination of the file, highlight the DRIVE field. Pressing ENTER will toggle between LIBRARY and DISK.

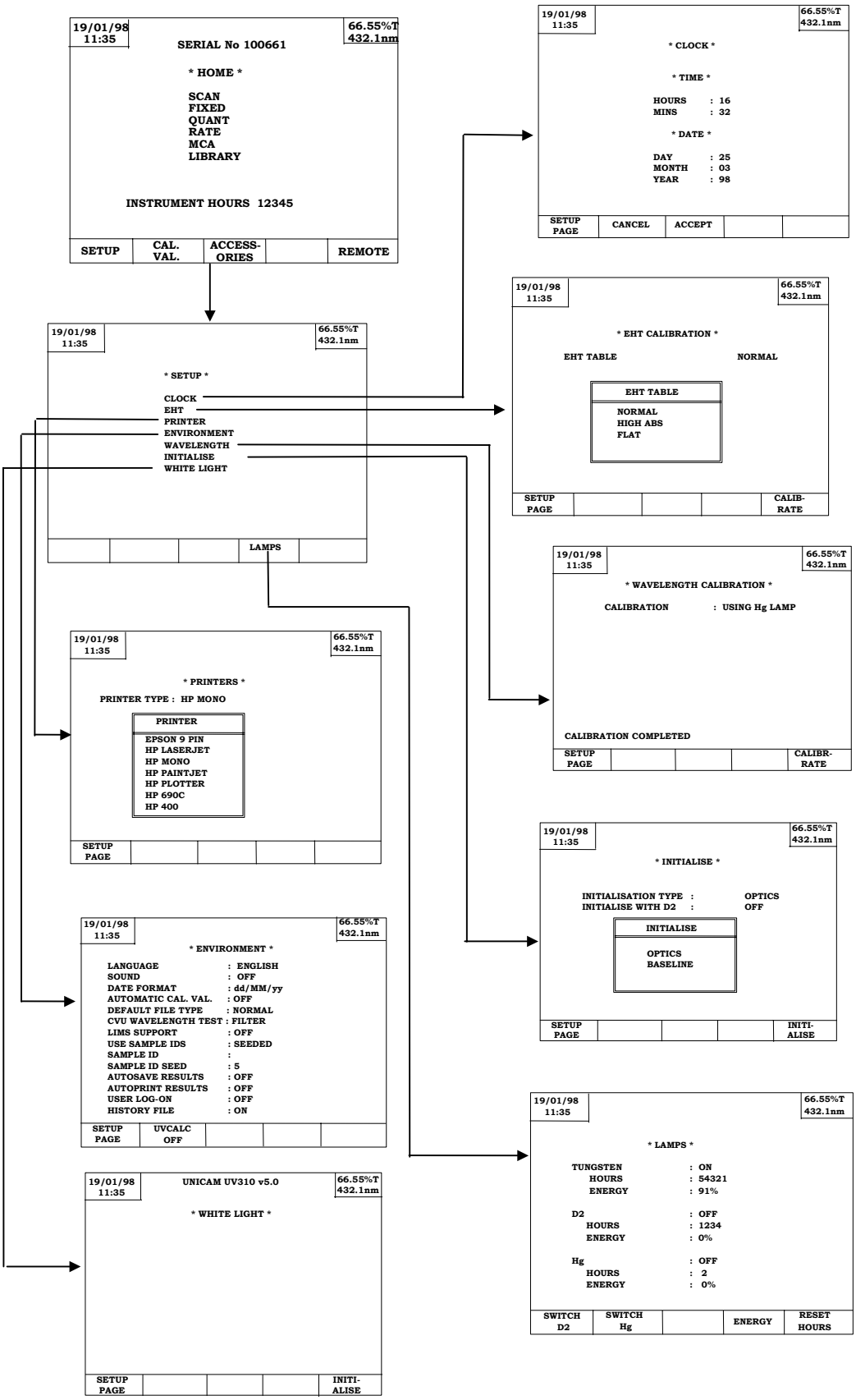


(←) - Acts as backspace and clears the last character in the line.

ACCEPT/SAVE - Accepts the edited field ready for saving. Only reads ACCEPT if edit is in progress.
SAVE - saves file to disk and is not present during an edit.

CANCEL - Abandons the naming operation. No files will be changed and the software returns to the calling screen.

SETUP


19/01/98 11:35
66.55%T 432.1nm
SERIAL No 100661
* HOME *
SCAN
FIXED
QUANT
RATE
MCA
LIBRARY
INSTRUMENT HOURS 12345
SETUP
CAL. VAL.
ACCESS-ORIES
REMOTE
* SETUP *
CLOCK
EHT
PRINTER
ENVIRONMENT
WAVELENGTH
INITIALISE
WHITE LIGHT
LAMPS
* CLOCK *
* TIME *
HOURS : 16
MINS : 32
* DATE *
DAY : 25
MONTH : 03
YEAR : 98
SETUP PAGE
CANCEL
ACCEPT
* EHT CALIBRATION *
EHT TABLE
NORMAL
EHT TABLE
NORMAL
HIGH ABS
FLAT
CALIB-RATE
* WAVELENGTH CALIBRATION *
CALIBRATION : USING Hg LAMP
CALIBRATION COMPLETED
CALIBR-RATE
* PRINTERS *
PRINTER TYPE : HP MONO
PRINTER
EPSON 9 PIN
HP LASERJET
HP MONO
HP PAINTJET
HP PLOTTER
HP 690C
HP 400
* ENVIRONMENT *
LANGUAGE : ENGLISH
SOUND : OFF
DATE FORMAT : dd/MM/yy
AUTOMATIC CAL. VAL. : OFF
DEFAULT FILE TYPE : NORMAL
CVU WAVELENGTH TEST : FILTER
LIMS SUPPORT : OFF
USE SAMPLE IDS : SEEDED
SAMPLE ID :
SAMPLE ID SEED : 5
AUTOSAVE RESULTS : OFF
AUTOPRINT RESULTS : OFF
USER LOG-ON : OFF
HISTORY FILE : ON
UVCALC OFF
* INITIALISE *
INITIALISATION TYPE : OPTICS
INITIALISE WITH D2 : OFF
INITIALISE
OPTICS
BASELINE
INITI-ALISE
UNICAM UV310 v5.0
* WHITE LIGHT *
* LAMPS *
TUNGSTEN : ON
HOURS : 54321
ENERGY : 91%
D2 : OFF
HOURS : 1234
ENERGY : 0%
Hg : OFF
HOURS : 2
ENERGY : 0%
SWITCH D2
SWITCH Hg
ENERGY
RESET HOURS

- This section describes how to set up the instrument.
- The main system setup options are available directly from the SETUP function key on the HOME page.

SETUP Page

- From the SETUP page move the cursor to the required option using the Up/Down Arrow keys. Select the option by pressing the ENTER key.

```
    * SETUP *

CLOCK
EHT
PRINTER
ENVIRONMENT
WAVELENGTH
INITIALISE
WHITE LIGHT
```

CLOCK : Switches to the CLOCK page.
EHT : Switches to the EHT CALIBRATION page.
PRINTER : Switches to the PRINTER page.
ENVIRONMENT : Switches to the ENVIRONMENT page.
WAVELENGTH : Switches to the WAVELENGTH CALIBRATION page.
INITIALISE : Switches to the OPTICAL INITIALISATION page.
WHITE LIGHT : Switches to the WHITE LIGHT Page.

To return to the HOME page press HOME.

CLOCK Page

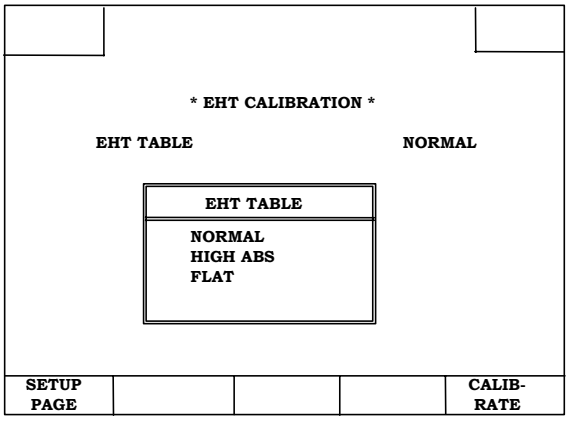
```
     * CLOCK *

     * TIME *

HOURS  :  16
MINS   :  32



     * DATE *

DAY    :  25
MONTH  :  12
YEAR   :  96
```

- From this page the internal spectrophotometer clock/calendar can be reset.
- To reset the time or date highlight the required parameter and press ENTER. Enter the new value using the number keys and press ENTER.
- Once all the parameters have been changed press ACCEPT.

The date or time will not be changed unless ACCEPT is pressed.

- CANCEL cancels the edit, leaving the previous values unchanged

EHT CALIBRATION Page



- This page is used to select and calibrate the EHT table used. The EHT table sets the amount of gain used at the photomultiplier detector, ensuring that the response of the detector is kept optimal across the wavelength range. If the EHT is set too low then the signal will be noisy; conversely, if the EHT is set too high then the detector will saturate.
- To select the EHT table press ENTER

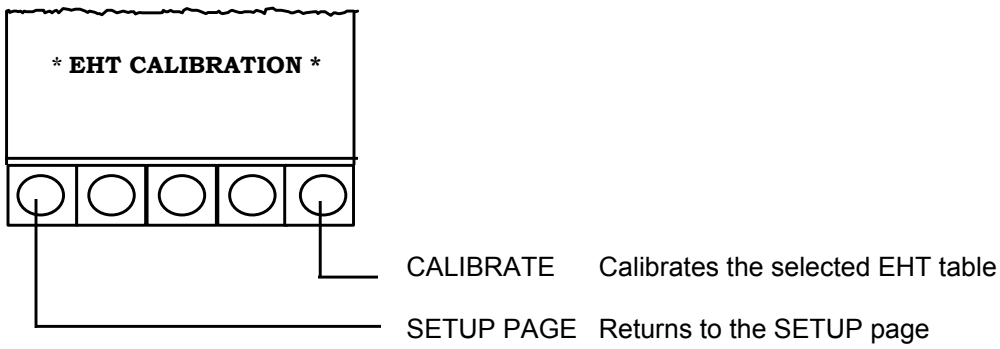
NORMAL This is the table for normal use.

HIGH ABS Use this table for highly attenuating accessories.

FLAT Use this table when scanning in intensity mode. Normally the EHT table compensates for variations in the source intensity. Consequently, use of the NORMAL or HIGH ABS options will result in major loss of detail in the intensity spectrum.

- To recalibrate any of the tables, first select the table to be calibrated and then press CALIBRATE.

CAUTION: DO NOT RECALIBRATE THE EHT TABLES UNLESS YOU ARE ABSOLUTELY SURE YOU NEED TO DO SO.



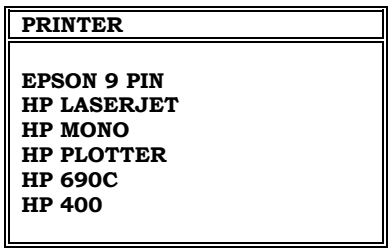
PRINTERS Page

- This page sets the system to work with the selected printer.

THE PRINTER MUST BE FITTED WITH A SERIAL INTERFACE

PRINTERS DESIGNED TO WORK ONLY IN A WINDOWS ENVIRONMENT ARE NOT COMPATIBLE WITH LOCAL CONTROL SOFTWARE

- The printer type is always highlighted. The default printer is HP Mono.To choose a printer press ENTER to display the list of supported printers, and select using cursor keys. Press ENTER to confirm entry.



Printer option	Supported Printers
EPSON 9 PIN	Epson 9 or 24 Pin Dot Matrix, using ESC/P language.
HP LASERJET	HP Laserjet Series
HP MONO	HP Deskjet 500 Series (and above) - Black & White
HP PLOTTER	Compatible with plotters using HPGL language.
HP 690C	HP Deskjet 690C – Colour
HP 400	HP Deskjet 400 - Mono

Printers not on the above list that claim Epson 9 pin / 24 pin / ESC/P or HP PCL (Programming Control Language) Level 3 compatibility should work with the instrument but are not guaranteed to do so and are therefore not supported. If in doubt contact your Thermo Electron approved Customer Support organization.

Before attempting to print using an external printer at any point during operation of the instrument, ensure that the printer is ready to print. Failure to do so will result in an error condition. Press CLEAR to clear the error message. Then rectify the problem with the printer, and try again.

ENVIRONMENT page

This page is used to select the language used for the software, the use of the beep, date format, and to enable/disable Automatic Calibration Validation and LIMS (Laboratory Information Management System) Support, to select the default filetype used when saving results, and to select whether wavelength calibration validation is carried out using the mercury lamp or glass filters in the CVU with the tungsten lamp.

```
    * ENVIRONMENT *

LANGUAGE                : ENGLISH
SOUND                   : OFF
DATE FORMAT             : dd/MM/yy
AUTOMATIC CAL. VAL.     : OFF
DEFAULT FILE TYPE       : NORMAL
CVU WAVELENGTH TEST     : FILTER
LIMS SUPPORT            : OFF
USE SAMPLE IDS          : OFF
AUTOSAVE RESULTS        : OFF
AUTOPRINT RESULTS       : OFF
USER LOG-ON             : OFF
HISTORY FILE            : OFF
```

LANGUAGE: Select from the list. The language used immediately changes to the one selected.

SOUND: Turns the warning beeper ON or OFF. If set to OFF then the only indication of any error is the screen message.

DATE FORMAT: Defaults to dd/MM/yy, but will toggle with ENTER to MM/dd/yy.

AUTOMATIC CAL. VAL. : Toggles between OFF and ON with Enter.

- When ON, and the CVU (Calibration Validation Unit) is fitted, the instrument automatically waits on start-up for the warm-up period (60 minutes) and then performs the Wavelength, Absorbance and Stray Light calibration tests (See CVU Section). Pressing Clear aborts the calibration.

DEFAULT FILE TYPE: Selects the default file type on the SAVE/RENAME page.

- Available formats are:

  NORMAL- The native file type used by the Local Control software
  CSV - Comma separated variable
  JCAMP-DX - JCAMP data exchange format

  Use up/down arrow keys to highlight choice and press ENTER to confirm selection.

CVU WAVELENGTH TEST: Toggles between Filter or Hg.

Selects the method used by the CVU (where fitted) to perform the Wavelength Accuracy Test.

LIMS SUPPORT: Toggles between **OFF** and **ON**.

- When **ON**, results, methods and sample IDs (when selected) are exported automatically after each measurement to the central LIMS computer via the RS232 port.

THIS INTERFACE MUST BE CONNECTED BEFORE LIMS SUPPORT IS ACTIVATED.

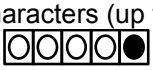
USE SAMPLE IDS : Choose between **OFF**, **SEEDED** and **PROMPT USER**.

- **OFF** - The system does not attach an identity to the sample.

- **SEEDED** - Enables the system to be set up to attach an identity to each sample automatically. This appears on the screen and the print-out. It is also exported to the LIMS (when enabled) with the results of the run and method used.

  Selection of **SEEDED** causes two additional items to appear in the Environment Menu:

  SAMPLE ID : Enter the name of the sample via the Text Entry Page.

  Use the Arrow keys to move the cursor to the required character and press ENTER. Once all the required characters (up to 11) have been entered press ACCEPT. If you make a mistake  will act as a backspace or CLEAR will clear the whole entry.

  SAMPLE ID SEED : Sets the number to be used for the first sample, via the numeric keypad.
  The Sample ID is incremented automatically **before** each run. Set the seed to zero for the results of the first run to be numbered 1.

- **PROMPT USER** - Before each run the Text Entry Page appears and the user is prompted to enter an identity for the sample.
  NOTE - a) When the Cell Programmer is used in AUTO mode the Sample ID is incremented automatically without stopping for ID confirmation between samples.
  b) PROMPT USER is not compatible with the Sipper used in Sip and Run or AutoSampler modes

AUTOSAVE RESULTS: Toggles between ON and OFF.

- When **ON,** results are saved automatically after each run. Selecting **ON** causes two additional items to appear in the Environment menu:

  FILENAME: Enter a filename of up to 5 characters via the Text Entry Page.

  FILE NUMBER: Enter a number between 0 and 999 via the numeric keypad. The number is appended to the filename and incremented automatically after each run.

AUTOPRINT RESULTS: Toggles between ON and OFF.

When **ON,** results are printed automatically after each run.

Before attempting to print at any point during operation of the instrument ensure that the printer is ready to print, ie switched on, on line and supplied with paper. Failure to do so will result in an error condition. Press Clear to clear the error message (the system may take a little time to respond). Ensure the printer is ready and retry.

USER LOG-ON: The default setting is OFF. Changing the setting to ON is password protected.

When set to **OFF,** any user has full access to all the functions of the instrument. When set to **ON,** users must identify themselves by user name and password at log-on, and then have access to whichever functions are enabled for them by the System Administrator.

Setting User Log-on to ON is password protected. Use the up and down arrow keys to move the highlight to **USER LOG-ON** and press Enter. This brings up the Text Entry Page. When the correct password is entered USER LOG-ON is set to ON, otherwise an error message is displayed, and it remains set to OFF. The default password is ADMIN. Note that the password is case sensitive, and in this password all the letters are upper case.

Logging on as ADMIN gives access to the system at Administrator level, and the CHANGE USERS function key is enabled.

*** CURRENT USERS ***

NAME	PASSWORD	PRIVILEGES E	C	F	I	H	L	B
ADMIN	ADMIN	√	√	√	√	√	√	√
----------	----------	–	–	–	–	–	–	–
----------	----------	–	–	–	–	–	–	–
----------	----------	–	–	–	–	–	–	–
----------	----------	–	–	–	–	–	–	–
----------	----------	–	–	–	–	–	–	–
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----------	----------	–	–	–	–	–	–	–
----------	----------	–	–	–	–	–	–	–
----------	----------	–	–	–	–	–	–	–

E = EDIT METHODS
C = CALIBRATIONS
F = DELETE FILES
I = INITIALISATIONS
H = HISTORY FILE
L = RESET LIFETIMES
B = DEFAULT BASELINE

CANCEL	ACCEPT		USERS 11 - 20	

Pressing the CHANGE USERS function key brings up the CURRENT USERS page. Up to 20 users can be listed by name and password. The privileges of each user can be set individually by the Administrator, and can be any combination of Edit Methods, Calibrations, Delete Files, Initialisations, History File, Reset Lifetimes, Default Baseline.

Only the Administrator is able to change passwords or edit the Current Users Page. It is strongly recommended that a new user name and password for the Administrator are set as soon as USER LOG-ON is activated, and that USER LOG-ON is activated whenever the instrument is to be used in a multi-user environment.

After USER LOG-ON is enabled, each time the instrument is powered up the user will be prompted to log on by entering name and password. At the close of a session the user logs off by pressing the LOG OFF function key on the Home Page, and choosing

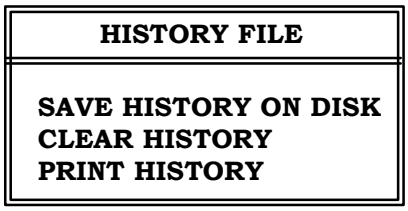
whether to PROCEED or STOP. When PROCEED is chosen the system waits for the next user to enter their name.

USER LOG-ON can be reset to OFF only by the Administrator. After USER LOG-ON has been set to OFF the list of users is cleared and the default User Name and Password are both reset to ADMIN.

HISTORY FILE: Toggles between ON and OFF.

The History File contains the history of the instrument. An entry is put into the file when there are changes to default baselines, wavelength calibrations, EHT calibrations, sipper calibrations and CVU tests, noting date, time and user. The file will also contain records of operations carried out by engineers during maintenance visits.

When **HISTORY FILE** is set to ON the HISTORY FILE function key becomes available on the Environment Page, unless USER LOG-ON is enabled and the user has been denied access by the Administrator. Pressing this function key brings up the History File Pop-up box.

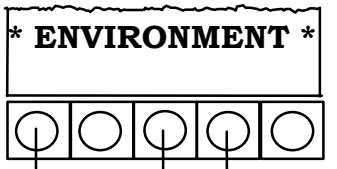


SAVE HISTORY ON DISK - The user is prompted for a file name and the instrument history is saved in CSV format which may be read by a suitable spreadsheet or text editor.

CLEAR HISTORY - Clears the Instrument History.

PRINT HISTORY - The Instrument History is printed out. *Make sure the printer is connected and ready before selecting PRINT HISTORY.*

The History File contains a maximum of 400 entries. When the number of entries reaches 390 a warning message is displayed, and it is necessary for the Administrator or a user with the History File privilege save to disk and/or print the existing history file, then clear the history file to make room for more entries.



HISTORY FILE - Appears when History File is enabled.

CHANGE USERS - Available only to Administrator when User Log-on enabled.

SETUP PAGE - Returns to the SETUP page.

WAVELENGTH CALIBRATION Page

```
* WAVELENGTH CALIBRATION *

CALIBRATION    :   USING D2 LAMP
```

- From this page the Wavelength calibration of the instrument can be adjusted.

CALIBRATION : Select between **USING HG LAMP** and **USING D2 LAMP**

WARNING: DO NOT ATTEMPT TO RECALIBRATE THE INSTRUMENT UNLESS YOU ARE ABSOLUTELY SURE YOU NEED TO DO SO. IF IN ANY DOUBT CONTACT THERMO ELECTRON APPROVED CUSTOMER SUPPORT.

To find out whether recalibration is needed it will be necessary to check the Wavelength Accuracy. This is most conveniently done with the optional CVU and Self Test Accessories.

Performing a Recalibration

ENSURE BOTH SAMPLE AND REFERENCE BEAMS ARE CLEAR BEFORE ATTEMPTING ANY WAVELENGTH CALIBRATION.

- There are two options, calibration with the optional Mercury lamp, or recalibration using the Deuterium lamp. Pressing ENTER toggles between them
- Press the **SETUP PAGE** function key to return to the SETUP page.
- Press the **CALIBRATE** function key to begin calibration. **STOP** becomes available during the calibration process. It stops the calibration process and leaves the existing calibration unchanged.

Mercury Lamp Calibration

- This option will optimise the wavelength calibration of the instrument by measuring the position of the emission lines of the mercury lamp and fitting the calibration accordingly. It can only be performed if the Mercury Lamp Accessory (Part Number 9423 UV9 0023E) is fitted and switched on. It should only be attempted if for any reason the instrument no longer achieves its quoted wavelength accuracy specification.
- The calibration will take at least 15 minutes. Once the calibration is complete the Default Baseline must be run.
- This operation will only need to be done if the existing calibration is corrupt, the grating has been replaced, or the monochromator drive has been replaced.
- Proceed as follows:

  Install the Mercury Lamp Accessory as detailed in the Mercury Lamp Accessory Installation and Maintenance Manual
  Ensure the Mercury Lamp is ON.
  Ensure the instrument is fully warmed up and the beams are clear.
  From WAVELENGTH CALIBRATION page select CALIBRATION USING Hg LAMP and press CALIBRATE.
  Once calibration is complete, switch both the Mercury Lamp and instrument OFF.
  Switch the instrument ON and allow to warm up.
  Run the Default Baseline.

Deuterium Lamp Calibration

- This option will optimise the wavelength calibration of the instrument by measuring the Deuterium lamp emission line at 656.1nm and fitting the calibration accordingly. It should only be attempted if for any reason the instrument no longer achieves its quoted wavelength accuracy specification.

- The calibration will take at least 10 minutes.

- Proceed as follows:
  Ensure Deuterium Lamp is ON.
  Ensure instrument is fully warmed up and the beams are clear.
  From WAVELENGTH CALIBRATION page press CALIBRATE.
  Once calibration is complete switch the instrument OFF.
  Switch instrument and Deuterium lamp ON and allow to warm up.
  Run Default Baseline as detailed below.

OPTICAL INITIALISATION Page

- This page is used to reset the instrument and define its initialisation and default baseline. These procedures ensure the optimum performance of the spectrophotometer.

INITIALISATION TYPE: When selected this displays a pop-up menu to choose between initialisation of optics or baseline.

OPTICS - During the normal initialisation procedure the spectrophotometer optimises the alignment of the lamp change mirror over a predefined range to give the maximum energy throughput. this operation defines the range over which the optimisation takes place. This should always be done when one of the lamps is changed.

BASELINE - This re-measures the default baseline. Ensure that both lamps are on and that the spectrophotometer is fully warmed up. This process will take about one hour.

The default baseline should be re-measured whenever one of the source lamps is changed or if the instrument is working at temperatures significantly different from 25 °C, or if the wavelength calibration is altered.

INITIALISE WITH D2 : This sets the instrument to initialise with or without the Deuterium lamp on. If set to ON then the instrument will automatically strike the Deuterium lamp during initialisation.

WHITE LIGHT Page

- The **WHITE LIGHT** feature is used to facilitate alignment of optical accessories in the sample compartment.

- When the **INITIALISE** function key is pressed the instrument will align the grating so that the zero order diffraction passes through the sample compartment. This provides a beam of white light which can be seen when a white card or similar is placed in the light path. In double beam instruments the action of the chopper causes the light to alternate between the sample and reference beams.

- When alignment is completed, pressing the **STOP** function key returns the grating to its normal position and pressing the **SETUP PAGE** function key returns to the Setup Page.

LAMPS Page

- The lamp functions are available directly from the LAMPS key on the SETUP page. If User Log-on is not in use, the HOME page will also have a LAMPS key.

- This page shows the status of the Tungsten Halogen, Deuterium and Mercury lamps, whether ON, OFF or FAILED, and their appropriate energy levels. It also allows the lamp hours to be reset and the Deuterium and Mercury lamps to be switched on or off.

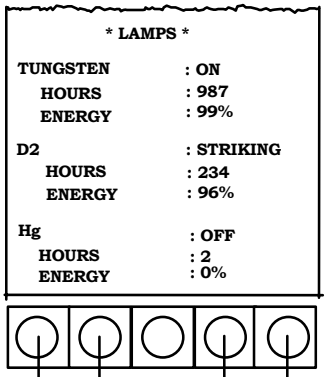
THE MERCURY LAMP SHOULD BE SWITCHED OFF WHEN NOT IN USE.

- The HOURS parameter states the number of hours that the lamp has been in use.

The Tungsten Halogen lamp should be replaced after 2000 hours. The Deuterium lamp should be replaced after 1000 hours.
Whenever a lamp is changed then the hours parameter should be reset to zero.

- The LAMP ENERGIES are measured as follows:

TUNGSTEN HALOGEN LAMP	-	Measured at 546 nm.
DEUTERIUM LAMP	-	Measured at 250 nm.
MERCURY LAMP	-	Measured at zero order.



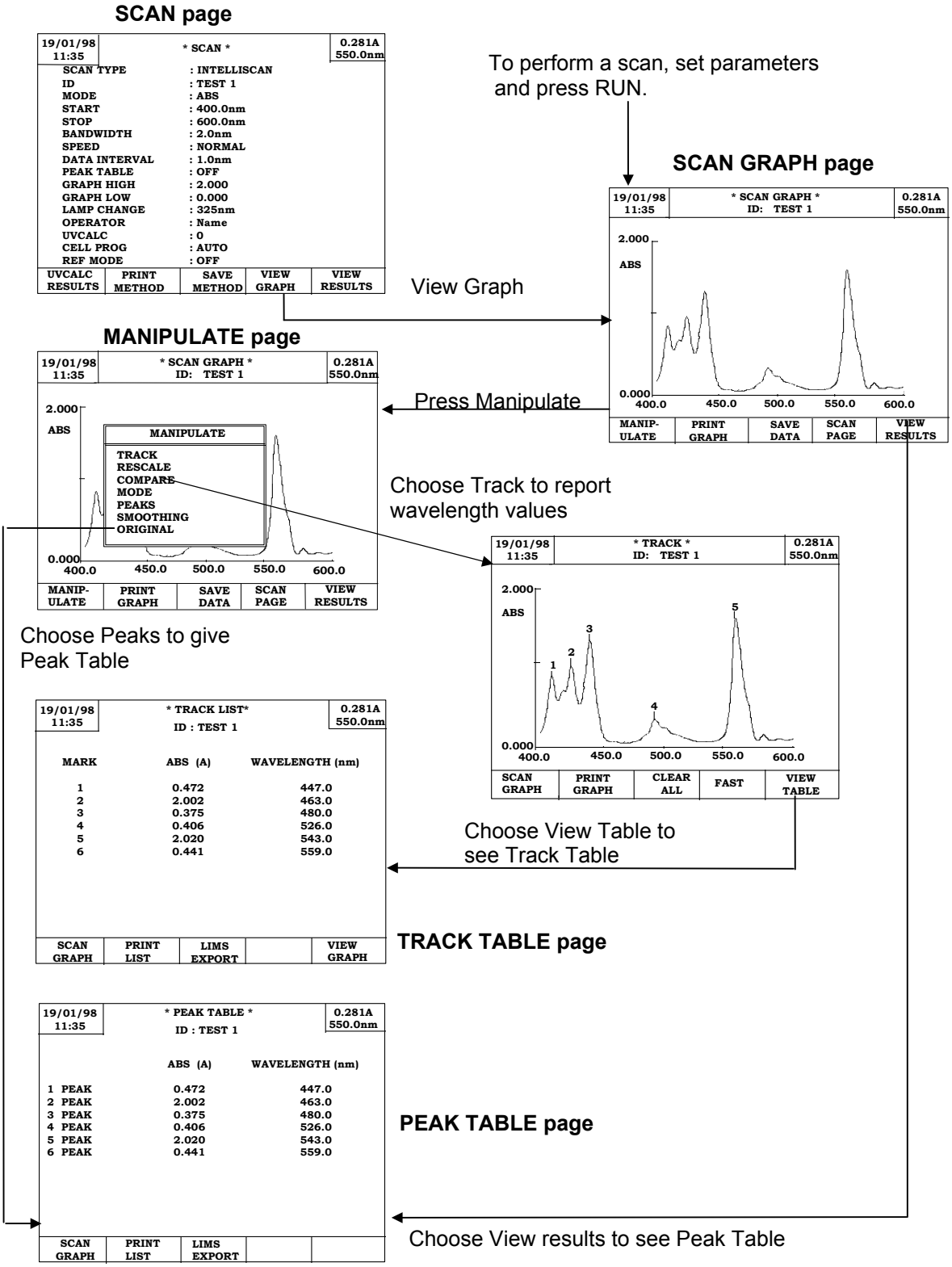
RESET HOURS – Displays a menu to choose whether the tungsten, deuterium or mercury lamp is to be reset. When selected resets hours and measures energy at the appropriate wavelength. **ALLOW THE LAMP AT LEAST 10 MINUTES TO WARM UP BEFORE RESETTING ITS HOURS.**

ENERGY - Displays a menu to choose whether the energy of the tungsten, deuterium or mercury lamp is to be measured. **ALLOW THE LAMP AT LEAST 10 MINUTES TO WARM UP BEFORE MEASURING ITS ENERGY. CLEAR BOTH SAMPLE AND REFERENCE BEAMS BEFORE MEASURING LAMP ENERGIES.**

SWITCH Hg – Switches the Mercury lamp ON or OFF depending on its current status.
THE MERCURY LAMP SHOULD BE TURNED OFF WHEN NOT IN USE.

SWITCH D2 -Turns the Deuterium lamp ON or OFF depending on its current status.

SCAN


SCAN page
19/01/98 11:35
* SCAN *
0.281A 550.0nm
SCAN TYPE : INTELLISCAN
ID : TEST 1
MODE : ABS
START : 400.0nm
STOP : 600.0nm
BANDWIDTH : 2.0nm
SPEED : NORMAL
DATA INTERVAL : 1.0nm
PEAK TABLE : OFF
GRAPH HIGH : 2.000
GRAPH LOW : 0.000
LAMP CHANGE : 325nm
OPERATOR : Name
UVCALC : 0
CELL PROG : AUTO
REF MODE : OFF
UVCALC RESULTS
PRINT METHOD
SAVE METHOD
VIEW GRAPH
VIEW RESULTS
To perform a scan, set parameters and press RUN.
SCAN GRAPH page
* SCAN GRAPH *
ID: TEST 1
2.000
ABS
0.000
400.0
450.0
500.0
550.0
600.0
MANIP-ULATE
PRINT GRAPH
SAVE DATA
SCAN PAGE
VIEW RESULTS
View Graph
MANIPULATE page
Press Manipulate
MANIPULATE
TRACK
RESCALE
COMPARE
MODE
PEAKS
SMOOTHING
ORIGINAL
Choose Track to report wavelength values
* TRACK *
ID: TEST 1
1
2
3
4
5
SCAN GRAPH
PRINT GRAPH
CLEAR ALL
FAST
VIEW TABLE
Choose Peaks to give Peak Table
* TRACK LIST*
ID : TEST 1
MARK ABS (A) WAVELENGTH (nm)
1 0.472 447.0
2 2.002 463.0
3 0.375 480.0
4 0.406 526.0
5 2.020 543.0
6 0.441 559.0
SCAN GRAPH
PRINT LIST
LIMS EXPORT
VIEW GRAPH
Choose View Table to see Track Table
TRACK TABLE page
* PEAK TABLE *
ID : TEST 1
ABS (A) WAVELENGTH (nm)
1 PEAK 0.472 447.0
2 PEAK 2.002 463.0
3 PEAK 0.375 480.0
4 PEAK 0.406 526.0
5 PEAK 2.020 543.0
6 PEAK 0.441 559.0
PEAK TABLE page
Choose View results to see Peak Table

- To select Scan highlight the SCAN option on the HOME PAGE and press ENTER. The SCAN Methods page is displayed and from here the instrument and analysis parameters can be set up.

- Move the cursor to the required parameter using the Up/Down Arrow keys. Press ENTER to enable a parameter to be changed.

- Once the method has been set up press ZERO/BASE to perform a baseline scan with the current method (see page 4) and then press RUN. The spectrophotometer will perform the scan and display the result on the SCAN GRAPH page. From here the spectrum can be manipulated and saved to Library or Disk. See LIBRARY for explanation of file functions.

SCAN PARAMETERS Page

Note: The current spectrum will be lost if any of the method parameters (except for the Operator name) are changed.

```
          * SCAN *
SCAN  TYPE              : INTELLISCAN

ID                      : TEST 1
MODE                    : ABS
START                   : 400.0  nm
STOP                    : 600.0  nm
BANDWIDTH               : 2.0  nm
SPEED                   : NORMAL
DATA INTERVAL           : 1.0  nm
PEAK TABLE              : OFF
GRAPH HIGH              : 2.000
GRAPH LOW               : 0.000
LAMP CHANGE             : 325  nm
OPERATOR                : Name
UVCALC                  : 0
CELL PROG               : AUTO
REF MODE                : OFF
```

SCAN TYPE : Select from STANDARD / INTELLISCAN.

- Standard mode enables the setting of a given scan speed and data interval. Intelliscan mode sets the data interval automatically and varies the scan speed according to the Absorbance of the spectrum.

ID : Enter a description using the TEXT ENTRY screen.

- The ID identifies the method and will be saved with the method and any spectra produced by the method.

MODE : Select from ABS / %T / I / 1D / 2D / 3D / 4D.

ABS	Selects Absorbance.
%T	Selects % transmittance
I	Selects Intensity mode. This will measure the intensity of the signal in the sample beam. *Note: Set the EHT table to FLAT when scanning in Intensity mode.*
1D	Selects first derivative. This records the first derivative of the Absorbance spectrum.
2D	Selects second derivative. This records the second derivative of the Absorbance spectrum.
3D	Selects third derivative. This records the third derivative of the Absorbance spectrum.
4D	Selects fourth derivative. This records the fourth derivative of the Absorbance spectrum.

The current spectrum will be lost if the Scan Mode is changed.

START: Selects start wavelength. *(190.0nm to 896.0nm)*

If the start wavelength requires the Deuterium lamp then this will be switched on. The Start wavelength must be at least 4 nm less than Stop wavelength. The current spectrum will be lost if the Start wavelength is changed.

STOP: Selects stop wavelength *(194.0nm to 900.0nm)*

The Stop wavelength must be at least 4 nm greater than the Start wavelength.
The current spectrum will be lost if the Stop wavelength is changed.

BANDWIDTH: Select from 4, 2, 1.5, 1, 0.5 and 0.2nm

SPEED : Selection depends on Scan Type selected.

- In Intelliscan mode select from ZIP / SURVEY / NORMAL / QUANT /HIGH RES / VERY HIGH RES.
- In Standard mode select from 3800, 2400, 1200, 600, 240, 120, 30, 10 or 1 nm per min.

DATA INTERVAL: Sets the frequency of data points in the spectrum. Selection depends on Scan Type.

In Intelliscan mode the data interval is fixed according to the intelliscan type selected.

Intelliscan	**Interval between points**
ZIP	4 nm
SURVEY	2 nm
NORMAL	1 nm
QUANT	0.5 nm
HIGH RES	0.2 nm
VERY HIGH RES	0.1 nm

In Standard mode the choice of data interval depends on the scan speed selected.

Speeds	Data Intervals
3800	4
2400	4, 2
1200	4, 2, 1
600	4, 2, 1, 0.5
240	4, 2, 1, 0.5, 0.2, 0.1
120	4, 2, 1, 0.5, 0.2, 0.1
30	4, 2, 1, 0.5, 0.2, 0.1
10	4, 2, 1, 0.5, 0.2, 0.1
1	4, 2, 1, 0.5, 0.2, 0.1

The current spectrum will be lost if the scan speed is changed.

PEAK TABLE: Select from OFF / PEAKS / VALLEYS / PKS & VALLEYS / ZERO CROSS / TRACK / RATIO, CORR RATIO, and PEAK HEIGHT

This selects the type of peak picking done automatically as part of the method. Results are reported on the Peaks Page. Peaks information is stored with any saved spectrum

OFF Sets Peak Table to Off. No peaks information is produced as part of the scan.

PEAKS Picks the highest peaks in a spectrum up to a maximum of 10 peaks

VALLEYS Picks the lowest troughs in a spectrum up to a maximum of 10 troughs.

PKS & VALLEYS Picks the 5 highest peaks and the 5 lowest valleys.

ZERO CROSS Picks all the points where the spectrum crosses zero up to a maximum of 10 crossing points.

TRACK This function allows the Absorbance (or other mode) values to be reported at up to 10 user selected wavelengths. To enter the desired wavelengths select PEAK TABLE I TRACK then press VIEW GRAPH.

You do not have to have a spectrum present on the graph to enter the selected wavelengths. Press MANIPULATE and select TRACK. For each wavelength move the cursor to the desired position press ENTER. Once all the wavelengths have been entered go back to the SCAN METHOD page and save the method.

RATIO This function allows the ratio λ_1/λ_2 to be automatically calculated at the end of the scan. To enter the desired wavelengths select PEAK TABLE and press ENTER then select RATIO. A pop up box appears in which to enter the first wavelength. Enter the desired wavelength

and press ENTER. Repeat for the second wavelength. Once all the method parameters have been set save the method.

CORR RATIO This function allows the ratio of two wavelengths to be calculated relative to a third wavelength $(\lambda_1-\lambda_3)/(\lambda_2-\lambda_3)$ automatically at the end of a scan. To enter the desired wavelengths select PEAK TABLE and press ENTER then select CORR RATIO. A pop up box appears in which to enter the first wavelength. Enter the desired wavelength and press ENTER. Repeat for the second and correction wavelengths. Once all the method parameters have been set save the method.

PEAK HEIGHT This function allows the height of a peak to be calculated relative to a local baseline rather than y = 0. To enter the desired

wavelengths select PEAK TABLE and press ENTER then select PEAK HEIGHT. A pop-up box appears in which to enter the wavelengths required.λ_1 and λ_3 define the baseline, λ_2 defines the peak. Once all the parameters have been set, save the method.

GRAPH HIGH: Select from range (GRAPH LOW + 0.01) to 6.00. Sets the upper graph limits on the SCAN GRAPH page.
GRAPH HIGH must be 0.01 greater than GRAPH LOW

GRAPH LOW: Select from range -0.3 to (GRAPH HIGH- 0.01).Sets the lower graph limits on the SCAN GRAPH page. *GRAPH LOW must be 0.01 less than GRAPH HIGH*

LAMP CHANGE: Select from 315, 320, 325, 330, 335, 340, D2, W, Hg.Selects the wavelength at which the source is changed between the Tungsten and Deuterium lamps.Selecting D2, W or Hg overrides any changeover and the selected lamp will be used regardless of the wavelength set.
THE MERCURY LAMP MUST BE SWITCHED OFF WHENEVER IT IS NOT IN USE

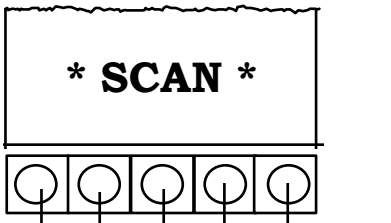
OPERATOR: Switches to the TEXT ENTRY screen.
The operator name is automatically saved with the method and any spectra produced by the method.
Changing the operator name will not cause the current spectrum to be lost.
If User Log-on is in operation, the operator name cannot be changed.

UVCALC: Switches to the UVCALC screen.

CELL PROG: Appears when the Cell Programmer is fitted. Switches to the CELL PROG screen.

REF MODE: Appears when the Cell Programmer is fitted. Toggles the status of the Cell Programmer reference mode

SCAN PARAMETERS page function keys



VIEW RESULTS - Switches to the Scan Peak Table screen if any of the peak functions have been performed or the Track Table screen if track has been used.

VIEW GRAPH - Switches to the Scan Graph screen.

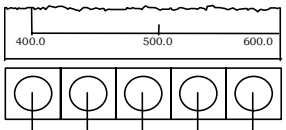
SAVE METHOD - Brings up the Filename Function screen and then saves the method including ID, operator name and track wavelengths if the PEAK TABLE parameter is set to TRACK.

PRINT METHOD - Prints the current method parameters on the printer

UVCALC RESULTS - Switches to UVCalc results screen if an equation has been entered and results are available.

SCAN GRAPH Page

- This page displays spectra and allows them to be manipulated.



VIEW RESULTS - Switches to the PEAK TABLE page.

SCAN PAGE - Returns to the SCAN page.

SAVE DATA - Displays the SAVE screen from where method and data can be saved to disk.

PRINT GRAPH - Provides a hardcopy of the results as shown on screen.

MANIPULATE - Displays the Manipulate options.

- Pressing RUN starts a scan using the current method.
- Pressing ZERO/BASE starts a baseline using the current method.

MANIPULATE OPTIONS

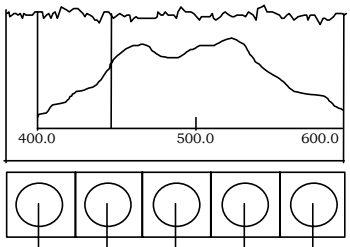
MANIPULATE
TRACK RESCALE COMPARE MODE PEAKS SMOOTHING ORIGINAL

TRACK	Reports x and y axis values using the tracking cursor.
RESCALE	Changes x and y axis scales automatically or manually.
COMPARE	Loads reference spectrum for comparison.
MODE	Changes mode. Select from %T / ABS / 1D / 2D / 3D / 4D.
PEAKS	Finds spectral peaks. Select from PEAKS / VALLEYS / PEAKS & VALLEYS/ ZERO CROSS / RATIO / CORR. RATIO / PK HEIGHT.
SMOOTHING	Applies LOW, MEDIUM or HIGH modified/improved Savitsky-Golay smoothing to the spectrum.
ORIGINAL	Resets the graph to display the data as originally collected.

TRACK

- To move the vertical cursor across the screen use the Left and Right Arrow keys. The cursor always moves to a data point regardless of the displayed scales. Pressing ENTER places a marker at the current wavelength. Up to 10 wavelengths can be selected.

TRACK page function keys



- Pressing CLEAR will delete markers in turn, highest number first.
- The x-axis values are listed on the TRACK table page. Further markers can be added to the spectrum at any time; however selecting TRACK will cause any previous PEAK TABLE information to be lost.

VIEW TABLE - Switches to the TRACK TABLE page.

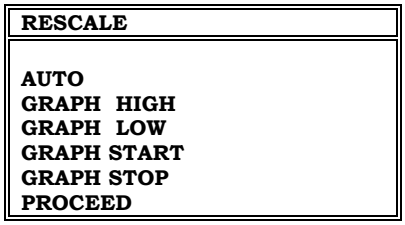
FAST/SLOW - Toggles between two cursor speeds. In FAST mode the cursor jumps 5% of the graph or to the next data point whichever is the greater. In SLOW mode the cursor jumps to the next data point or the next display pixel whichever is the greater. The function key label shows the next speed ie the opposite to the one selected.

CLEAR ALL - Clears all the markers and the TRACK TABLE.

PRINT GRAPH - Provides a hardcopy of the results showing the markers and x and y-axis values.

SCAN GRAPH - Returns to the SCAN GRAPH page.

RESCALE



- This option gives pop-up menus for changing the graph x and y -axis scales.
- Move the cursor to one of the options and press ENTER to select an operation.

AUTO	Displays the SCAN GRAPH with the x and y-axes rescaled so that the Spectrum fills the screen.
GRAPH HIGH	Pops up a window for entry of the GRAPH HIGH limit.
GRAPH LOW	Pops up a window for entry of the GRAPH LOW limit.
GRAPH START	Pops up a window for entry of the required start wavelength.
GRAPH STOP	Pops up a window for entry of the required stop wavelength.
PROCEED	Used after GRAPH HIGH, GRAPH LOW, GRAPH START or GRAPH STOP to return to the SCAN GRAPH page with the graph rescaled using the new parameters.

COMPARE

- When selected, Compare goes to the LIBRARY page and displays a list of scan data files. Highlight the desired file using the Up/Down Arrow keys and press LOAD. The reference spectrum is displayed as a dotted trace.
- Once loaded the reference spectrum will remain on the screen (and will be printed) with all subsequent scans until removed. To remove the reference spectrum from the display, select MANIPULATE ORIGINAL or load a new method.

MODE: Select from ABS / %T / 1D / 2D / 3D / 4D.

ABS	Selects Absorbance.
%T	Selects % transmittance.
1D	Selects first derivative. This records the first derivative of the Absorbance spectrum.
2D	Selects second derivative. This records the second derivative of the Absorbance spectrum.
3D	Selects third derivative. This records the third derivative of the Absorbance spectrum.
4D	Selects fourth derivative. This records the fourth derivative of the Absorbance spectrum.

PEAKS

FUNCTION
PEAKS VALLEYS PKS & VALLEYS ZERO CROSS RATIO CORR RATIO PK. HEIGHT

- This option enables the spectrum to be automatically searched for peaks, valleys or zero crossing points. Move the cursor to one of the options and press ENTER to perform a search. When the search is complete the spectrum is displayed with the peak positions marked. For a peak to be found there must be more than 15 data points between that point and a previous peak.

For RATIO and CORR RATIO enter the wavelengths as prompted. All results can be viewed by pressing ○○○○● VIEW RESULTS.

PEAKS	Marks the 10 highest peaks.
VALLEYS	Marks the 10 lowest valleys.
PKS&VALLEYS	Marks the 5 highest peaks and 5 lowest valleys.
ZERO CROSS	Marks the first 10 zero crossings
RATIO	Calculates the ratio λ_1/λ_2
CORR RATIO	Calculates the ratio $(\lambda_1-\lambda_3)/(\lambda_2-\lambda_3)$.
PK HEIGHT	Calculates the peak maximum relative to a local baseline.

SMOOTHING

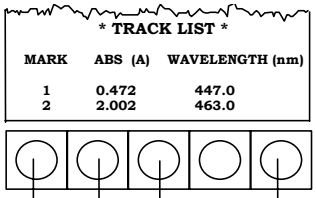
- This option offers a pop-up menu to choose one of three smoothing algorithms. Choices are NONE, LOW, MEDIUM and HIGH. A Savitsky-Golay smooth is performed on the data and in each case data points will be lost from either end of the data.

SMOOTHING	No of POINTS USED	POINTS LOST AT EACH END
NONE	0	0
LOW	9	4
MEDIUM	17	8
HIGH	33	16

ORIGINAL

- This removes any manipulation and displays the spectrum as originally collected and specified by the scan method. It will also clear any Compare spectrum.

TRACK TABLE Page



- The list shows the y-axis values of the spectrum for the wavelengths marked during TRACK. The measured values will be ABS, %T, INTENSITY or 1D / 2D / 3D / 4D depending on the current mode.

VIEW GRAPH - Switches to the TRACK page.

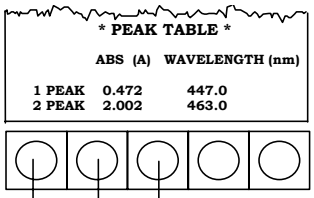
LIMS EXPORT – Sends the results via the RS232 port.

PRINT LIST - Prints the list on the selected printer.

SCAN GRAPH - Returns to the SCAN GRAPH page.

- If a spectrum is saved then the track markers are also saved and will be displayed when the spectrum is reloaded.

PEAK TABLE Page



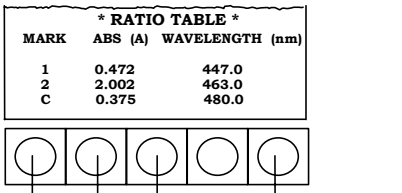
- The list shows the positions and values of the peaks as calculated by the function selected in MANIPULATE PEAKS. The measured values will be ABS, %T, INTENSITY or 1D / 2D / 3D / 4D depending on the current mode and are sorted by wavelength. Each marker is identified as a peak, valley or zero crossing.

LIMS EXPORT – Sends the results via the RS232 port.

PRINT LIST - Prints the list on the selected printer.

SCAN GRAPH - Returns to the SCAN GRAPH page.

RATIO TABLE Page



- The page shows the positions and values of the wavelengths and the ratio as selected by the RATIO or CORR RATIO functions.

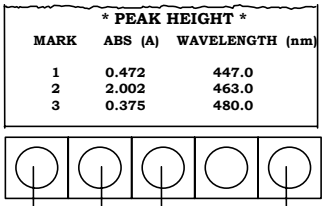
VIEW GRAPH - Returns to the SCAN GRAPH page.

LIMS EXPORT – Sends the results via the RS232 port

PRINT LIST - Prints the list on the selected printer.

SCAN GRAPH - Returns to the SCAN GRAPH page.

PEAK HEIGHT Page



- This page shows the position and values of the wavelengths and the peak height as selected by the PEAK HEIGHT function.

VIEW GRAPH - Returns to the SCAN GRAPH page.

LIMS EXPORT – Sends results via the RS232 port.

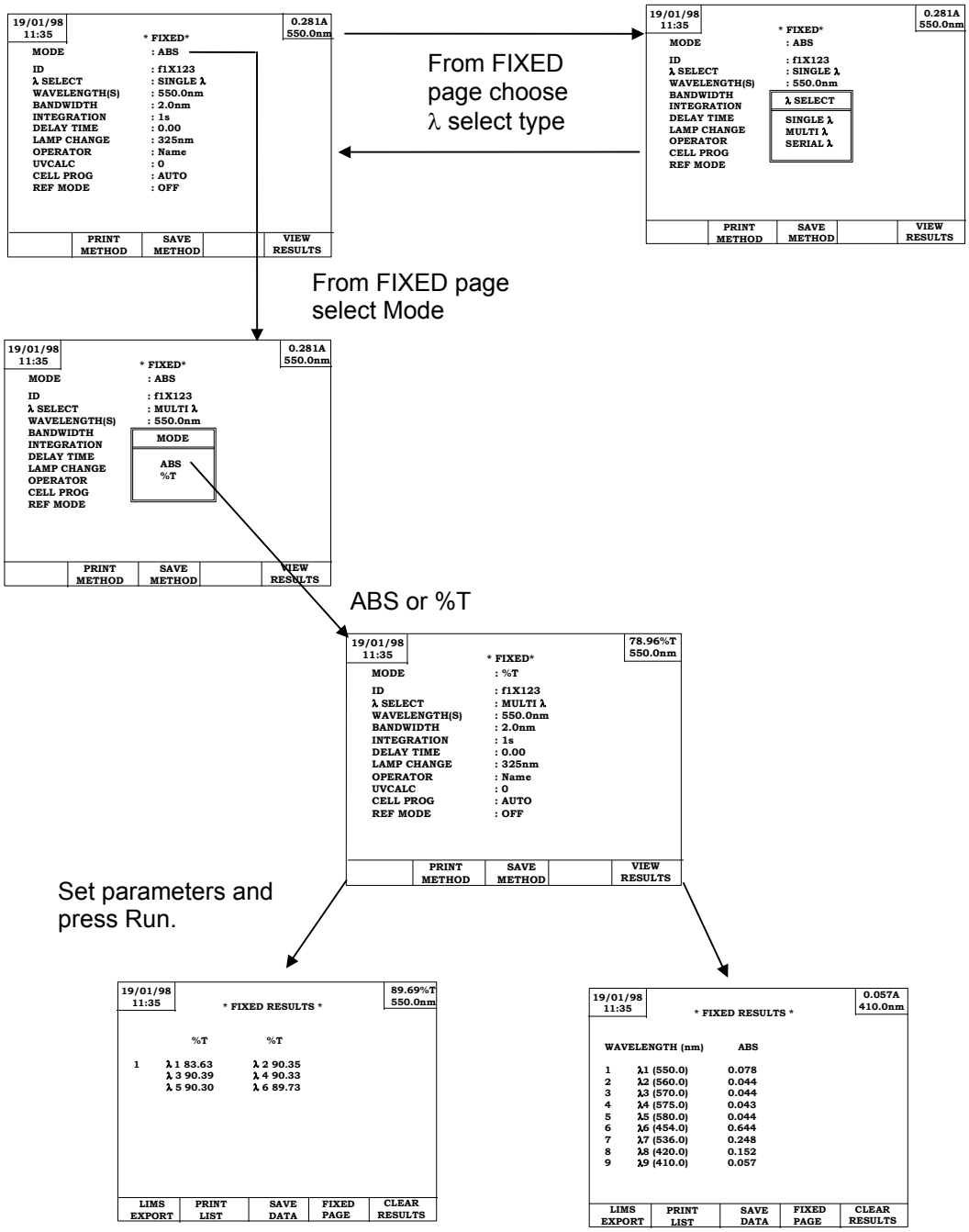
PRINT LIST - Prints the list on the selected printer.

SCAN GRAPH - Returns to the SCAN GRAPH page.

This page is intentionally left blank

FIXED

FIXED Page



- Instrument and analysis parameters are set up on the FIXED page. Move the cursor to the required parameter using the Up/Down Arrow keys. Change the parameter by pressing the ENTER key.
- Once the method has been set up press ZERO/BASE to zero the instrument for the current method (See page 4) and press RUN. The spectrophotometer will perform a measurement and display the result on the FIXED RESULTS page.
- Once all results have been collected, save the data.

FIXED METHOD Page

```
          * FIXED *
MODE                : ABS

ID                  :
λ SELECT            : SINGLE λ
WAVELENGTH(S)       : 550.0 nm
BANDWIDTH           : 2.0 nm
INTEGRATION         : 1 s
DELAY TIME          : 00:00
LAMP CHANGE         : 325 nm
OPERATOR            :
UVCALC              : 0
CELL PROG           : AUTO
REF MODE            : OFF
```

MODE : Select from ABS / %T.

ABS	Selects Absorbance.
%T	Selects % transmittance.

ID: Enter a description using the TEXT ENTRY screen.

- The ID identifies the method and will be saved with the method and any results produced by the method.

λ SELECT: Select from SINGLE λ /MULTI λ /SERIAL λ.

SINGLE λ	This option is used to measure each sample at a single wavelength which is the same for each sample.
MULTI λ	This option allows each sample to be measured at up to 20 wavelengths, which are the same for each sample.
SERIAL λ	This option allows a single wavelength measurement to be made at a different wavelength on up to 9 samples.

WAVELENGTH(S):

SINGLE λ Use the numeric key pad to enter the required wavelength into the pop-up box. Press ENTER when finished.

MULTI λ Use the up and down arrow keys to move to the wavelength to be entered or edited and press ENTER to display the edit box. Use the numeric keypad to enter the wavelength and press ENTER when finished. The instrument returns to the MULTI λ screen with the next wavelength in the list highlighted. Up to 20 wavelengths may be entered. When the list is finished press the ACCEPT function key to accept the new list or the CANCEL function key to return to the FIXED METHOD page without changing the wavelength list.

SERIAL λ Press ENTER to display the edit box for the wavelength to be used for the first sample. Data entry is as for MULTI λ above. When the required wavelengths have been entered press ACCEPT to accept the new list, or press CANCEL to return to the FIXED METHOD page leaving the original list unchanged.

The available wavelength range is 190.0nm to 900.0nm

If the wavelength requires the Deuterium lamp then this will be switched on. The current data will be lost if the wavelength is changed.

BANDWIDTH: Select from 4, 2, 1.5, 1, 0.5 and 0.2nm

INTEGRATION: Enter integration time in seconds.

- This sets the integration time for which the result is measured.

The current data will be lost if the integration time is changed.

DELAY TIME: Set a time in the range 00.05 to 99.59,using . to separate minutes and seconds.

- This sets the time between pressing RUN and the start of the measurement. The range is from 0 to 99 minutes and 59 seconds.

LAMP CHANGE: Select from 315, 320, 325, 330, 335, 340, D2, W, Hg.

- Selects the wavelength at which the source is changed between the Tungsten and Deuterium lamps.Selecting D2, W or Hg overrides any changeover and the selected lamp will be used regardless of the wavelength set.

THE MERCURY LAMP MUST BE SWITCHED OFF WHENEVER IT IS NOT IN USE

OPERATOR: Switches to the TEXT ENTRY screen.

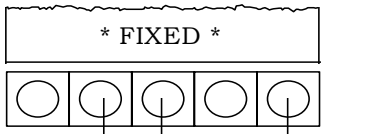
- The operator name is automatically saved with the method and any data produced by the method.

Changing the operator name will not cause any current data to be lost.
N.B. If user log-on is in operation, the operator name cannot be changed.

UVCALC: Switches to the UVCALC screen.

CELL PROG: Switches to the CELL PROG. screen (if fitted).
REF MODE: Toggles the status of the Cell Programmer reference mode (if fitted).

FIXED Method Page Function Keys



VIEW RESULTS - Switches to the FIXED RESULTS page.

SAVE METHOD - Brings up the SAVE page from where the method can be saved to Disk.

PRINT METHOD - Prints the current method parameters on the printer.

- Pressing RUN starts a fixed measurement using the current method and switches to the FIXED RESULTS page.
- Pressing ZERO starts a zero using the current method.

Any changes to the WAVELENGTH, BANDWIDTH, INTEGRATION or LAMP CHANGE parameters will invalidate the current results.

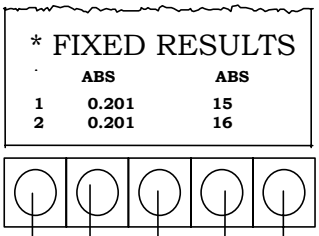
If AUTOPRINTING is selected (see SETUP for details), a change to the MODE parameter will invalidate the current results.

FIXED RESULTS Page

- The layout of the page depends on the Mode and λ Select in use.

SINGLE λ	Up to 2 columns of results are displayed per page. Results accumulate on the same page until it is full.
MULTI λ	Two columns of results are displayed per page. Results of each sample always start on a new page.
SERIAL λ	One column of results is displayed per page. Results accumulate on the same page until it is full.

- To move up or down pages of results use the Up/Down arrow keys.
- Results are numbered sequentially from 1 to 600.



CLEAR RESULTS - All results are cleared ready for the start of the next batch.

FIXED PAGE - Returns to the FIXED METHOD page.

SAVE DATA - Brings up the SAVE page from where the results can be saved to Disk.

PRINT LIST - Prints the list on the selected printer.

LIMS EXPORT – Sends the results via the RS232 port.

- Press RUN to take another sample measurement.
- Press ZERO/BASE to zero the instrument at the wavelength(s) specified in the method.

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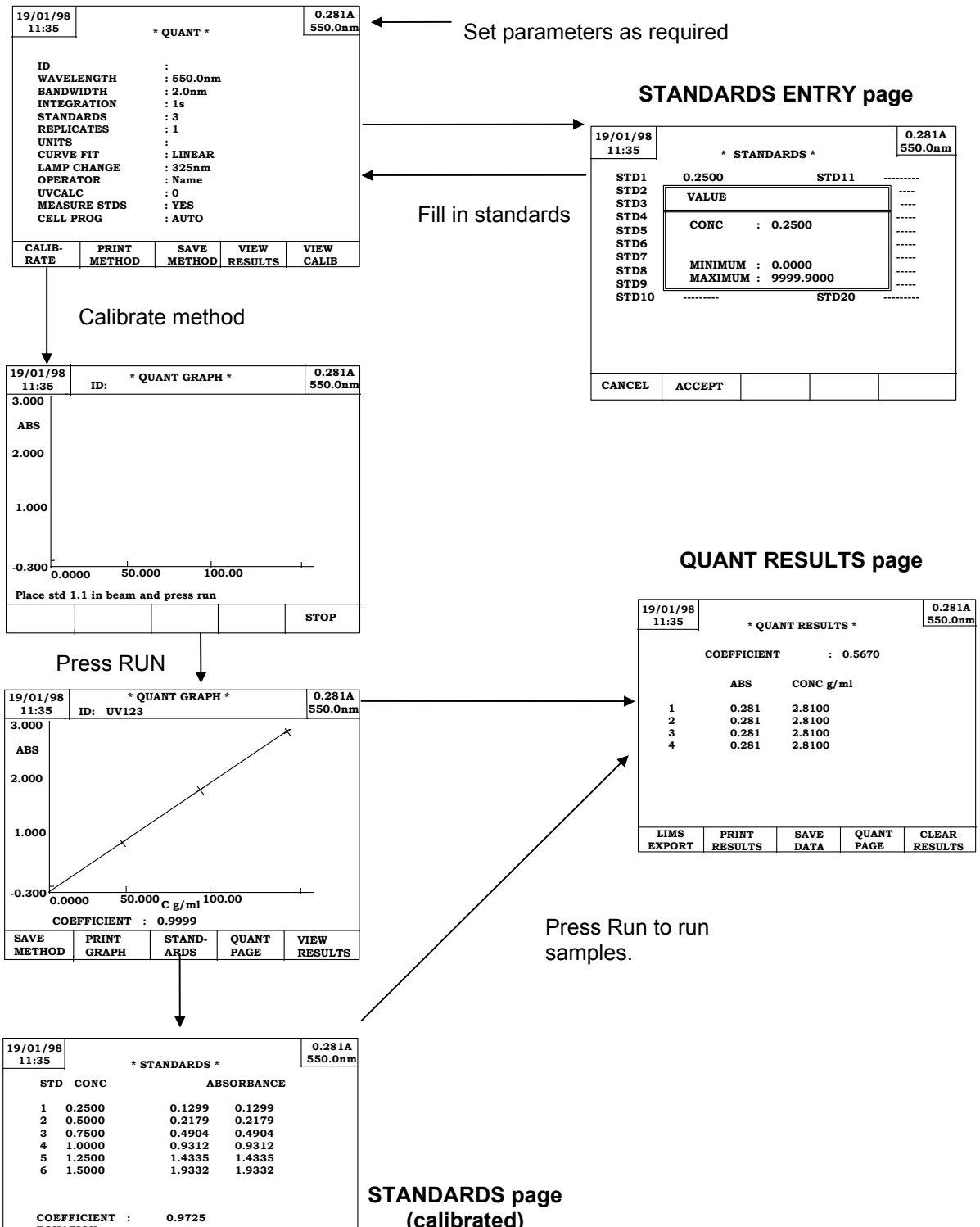
QUANT

QUANT page



STANDARDS page (calibrated)

Instrument and analysis parameters are set up on the QUANT page. Move the cursor to the required parameter using the Up/Down Arrow keys. Change the parameter by pressing the ENTER key.

- Once all results have been collected, save the data.

QUANT METHOD Page

```
          * QUANT *

ID                    :
WAVELENGTH            : 550.0 nm
BANDWIDTH             : 2.0 nm
INTEGRATION           : 1 s
STANDARDS             : 3
REPLICATES            : 1
UNITS                 :
CURVE FIT             : LINEAR
LAMP CHANGE           : 325 nm
OPERATOR              :
UVCALC                : 0
MEASURE STDS          : YES
CELL PROG             : AUTO
REF MODE              : OFF
```

ID: Enter a description using the TEXT ENTRY screen.

- The ID identifies the method and will be saved with the method and any results produced by the method.

WAVELENGTH: The available wavelength range is 190.0nm to 900.0nm

If the wavelength requires the Deuterium lamp then this will be switched on. The current data will be lost if the wavelength is changed.

BANDWIDTH: Select from 4, 2, 1.5, 1, 0.5 and 0.2nm

INTEGRATION: Enter integration time in seconds.

This sets the integration time for which the result is measured.
The current data will be lost if the integration time is changed.

STANDARDS: Brings up the Standards Entry Page

- Use the up and down arrow keys to move through the list of standards. When the standard to be entered or edited is highlighted, press ENTER to display the Edit pop-up. Use the numeric keys to enter the concentration of the standard and press ENTER when finished. The instrument returns to the Standards Entry page with the highlight on the next standard on the list. Up to 20 standards can be specified.

Changing the standards will cause any current data to be lost.

REPLICATES: Enter number of replicates for each standard.

- Sets the number of times each standard is measured (maximum 3). Each value obtained is used in the calibration.

UNITS: Enter units for concentration using the TEXT ENTRY page.
CURVE FIT: Select from LINEAR / LINEAR TO 0 / QUADRATIC / QUAD TO 0.

- Selects the curve fit algorithm used in the calibration.

LINEAR	performs a linear calibration. At least two standards are required.
LINEAR TO 0	performs a linear calibration forced through zero. At least one standard is required
QUADRATIC	performs a quadratic fit on the data. At least three standards are required.
QUAD TO 0	performs a quadratic fit with the data forced through zero. At least two standards are required.

Changing the curve fit will cause the existing calibration to be recalculated.
Any results associated with the previous calibration will be lost.

LAMP CHANGE: Select from 315, 320, 325, 330, 335, 340, D2, W, Hg.

Selects the wavelength at which the source is changed between the Tungsten and Deuterium lamps. Selecting D2, W or Hg overrides any changeover and the selected lamp will be used regardless of the wavelength set.

THE MERCURY LAMP MUST BE SWITCHED OFF WHENEVER IT IS NOT IN USE
Any current data will be lost if the lamp changeover wavelength is changed

OPERATOR: Switches to the TEXT ENTRY screen.

The operator name is automatically saved with the method and any data produced by the method.
Changing the operator name will not cause any current data to be lost.
If User Log-on is in operation, the operator name cannot be changed.

UVCALC: Switches to the UVCALC screen.

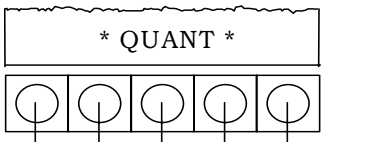
MEASURE STDS: Toggles between YES and NO.

- When YES, and Standard concentrations have been entered from the Quant Standards page, pressing Calibrate causes the instrument to prompt the user to put the standard in the beam and press Run to measure, for each Standard in turn.
- When NO, pressing Calibrate causes the system to prompt for an absorbance to be entered manually for each Standard, effectively enabling a calibration originating elsewhere to be entered.

CELL PROG : Switches to the CELL PROG. screen (if fitted).

REF MODE: Toggles the status of the Cell Programmer Reference Mode (if fitted).

QUANT Page function keys



VIEW CALIB - Switches to the QUANT GRAPH page if a valid calibration exists.

VIEW RESULTS - Switches to the Quant Results page if there are any sample results.

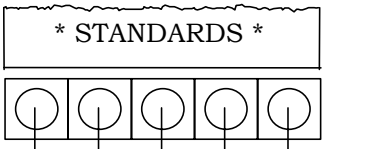
SAVE METHOD - Brings up the SAVE page from where the method can be saved to Library or Disk.

PRINT METHOD - Prints the current method parameters and the standards table on the printer.

CALIBRATE - Switches to the Standards Entry page.

QUANT STANDARDS Page

- This page lists the standards as defined in the QUANT METHOD. Before the system can be calibrated each standard must have a concentration entered.
- To enter Standard concentrations use the up and down arrow keys to move through the list of standards. When the standard to be entered or edited is highlighted press ENTER to display the Edit pop-up. Use the numeric keys to enter the concentration of the standard and press ENTER when finished. The instrument returns to the Standards Entry Page with the highlight on the next standard on the list. Up to 20 standards can be specified. When all the standards have been entered, press the ACCEPT function key to return to the QUANT Page with the new list of standards, or CANCEL to return leaving the old list unchanged.
- If a calibration has been done then the correlation coefficient and the equation are displayed.
- If a calibration has not been done pressing RUN causes the warning prompt "CANNOT RUN WITHOUT CALIBRATION" to appear, otherwise it takes a sample measurement and switches to the Quant Results screen. Pressing ZERO/BASE starts a zero using the current method.



VIEW CALIB - Switches to the QUANT GRAPH page if a valid calibration exists

VIEW RESULTS - Switches to the QUANT RESULTS page if there are any results in the table.

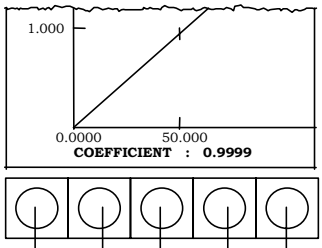
QUANT PAGE - Switches back to the Quant page.

EDIT STD – Available after calibration. Allows each standard to be used, ignored or remeasured.

EDIT CURVE – Available after calibration. Allows curve fit to be changed.

QUANT CALIBRATION

- Press ZERO/BASE to zero the instrument with the current method.
- To calibrate the system press return to the QUANT page and press CALIBRATE. The QUANT CALIBRATION graph will be displayed and the instrument will prompt for each standard (and replicate) in turn. As the measurements of the standards proceed the datapoints are marked on the graph. When all the standards have been measured the system calculates the equation, rescales the graph then draws and displays the line of best fit on the graph.
- A calibration can be stopped by pressing the STOP function key. The calibration will be aborted and the software will return to the QUANT STANDARDS page. Any values obtained will be lost.
- If a calibration has not been done pressing RUN causes the warning prompt "CANNOT RUN WITHOUT CALIBRATION" to appear, otherwise it takes a sample measurement and switches to the Quant Results screen.



VIEW RESULTS - Switches to the Quant Results page if there are results.

QUANT PAGE - Switches back to the Quant page.

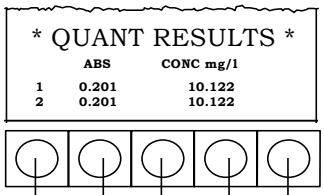
STANDARDS - Switches to the Quant Standards page.

PRINT GRAPH - Prints the Quant method and calibration graph.

SAVE METHOD - Switches to the SAVE page.

QUANT RESULTS Page

- To view further pages of results use the Up and Down arrow keys.
- Pressing RUN takes another sample measurement and displays the result.
- Results are numbered sequentially and any batch can be of up to 600 samples.



CLEAR RESULTS - Deletes all results from the results table.

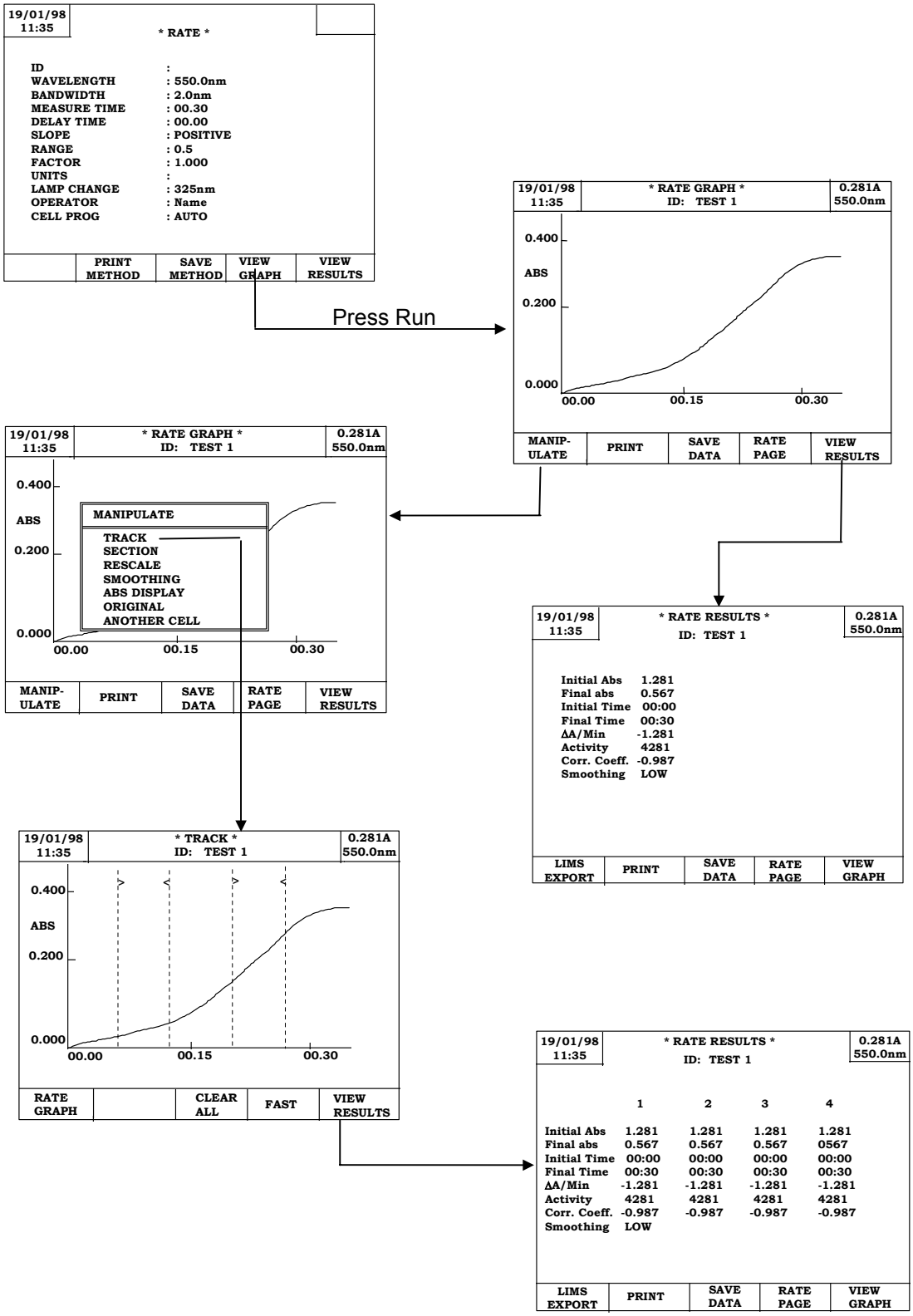
QUANT PAGE - Switches back to the Quant page.

SAVE DATA - Brings up the SAVE page.

PRINT LIST - Gives a printout of the results.

LIMS EXPORT– Sends the results via the RS232 port.

RATE


19/01/98 11:35
* RATE *
ID :
WAVELENGTH : 550.0nm
BANDWIDTH : 2.0nm
MEASURE TIME : 00.30
DELAY TIME : 00.00
SLOPE : POSITIVE
RANGE : 0.5
FACTOR : 1.000
UNITS :
LAMP CHANGE : 325nm
OPERATOR : Name
CELL PROG : AUTO
PRINT METHOD
SAVE METHOD
VIEW GRAPH
VIEW RESULTS
Press Run
19/01/98 11:35
* RATE GRAPH *
ID: TEST 1
0.281A
550.0nm
0.400
ABS
0.200
0.000
00.00
00.15
00.30
MANIP-ULATE
PRINT
SAVE DATA
RATE PAGE
VIEW RESULTS
MANIPULATE
TRACK
SECTION
RESCALE
SMOOTHING
ABS DISPLAY
ORIGINAL
ANOTHER CELL
19/01/98 11:35
* RATE RESULTS *
ID: TEST 1
0.281A
550.0nm
Initial Abs 1.281
Final abs 0.567
Initial Time 00:00
Final Time 00:30
ΔA/Min -1.281
Activity 4281
Corr. Coeff. -0.987
Smoothing LOW
LIMS EXPORT
PRINT
SAVE DATA
RATE PAGE
VIEW GRAPH
19/01/98 11:35
* TRACK *
ID: TEST 1
0.281A
550.0nm
RATE GRAPH
CLEAR ALL
FAST
VIEW RESULTS
19/01/98 11:35
* RATE RESULTS *
ID: TEST 1
0.281A
550.0nm
1 2 3 4
Initial Abs 1.281 1.281 1.281 1.281
Final abs 0.567 0.567 0.567 0567
Initial Time 00:00 00:00 00:00 00:00
Final Time 00:30 00:30 00:30 00:30
ΔA/Min -1.281 -1.281 -1.281 -1.281
Activity 4281 4281 4281 4281
Corr. Coeff. -0.987 -0.987 -0.987 -0.987
Smoothing LOW
LIMS EXPORT
PRINT
SAVE DATA
RATE PAGE
VIEW GRAPH

- To select Rate highlight the RATE option on the HOME PAGE and press ENTER. The RATE Methods page is displayed and from here the instrument and analysis parameters can be set up.

- Move the cursor to the required parameter using the Up/Down Arrow keys. Press ENTER to enable a parameter to be changed.

- Once the method has been set up press RUN. The spectrophotometer will perform the rate and display the result on the RATE GRAPH page. From here the data can be manipulated and saved to Disk.

RATE PARAMETERS Page

Note: The current data will be lost if any of the method parameters (except for the ID, Slope, Factor, Units and Operator name) are changed.

```
          * RATE
*
ID                    : TEST 1
WAVELENGTH            : 340.0 nm
BANDWIDTH             : 2.0 nm
MEASURE TIME          : 00:30
DELAY TIME            : 00:00
SLOPE                 : POSITIVE
RANGE                 : 0.5
FACTOR                : 1.000
UNITS                 : I/U
LAMP CHANGE           : 325 nm
OPERATOR              : Name
CELL PROG             : AUTO
REF MODE              : OFF
```

ID: Enter a description using the TEXT ENTRY screen.

- The ID identifies the method and will be saved with the method and any results produced by the method.

WAVELENGTH: The available wavelength range is 190.0nm to 900.0nm

If the wavelength requires the Deuterium lamp then this will be switched on. The current data will be lost if the wavelength is changed.

BANDWIDTH: Select from 4, 2, 1.5, 1, 0.5 and 0.2nm

MEASURE TIME: Set a time in the range 00:05 to 99:59.

- This sets the time over which the sample will be measured. The range is from 5 seconds to 99 minutes and 59 seconds in steps of 1 second.

- If the cell programmer is ON then the measurement time sets the time between individual measurements on the first cell (i.e. the time for each cycle).

DELAY TIME: Set a time in the range 00:05 to 99:59.

- This sets the time between pressing RUN and the start of the measurement. The range is from 0 to 99 minutes and 59 seconds in steps of 1 second.

SLOPE: Select from POSITIVE or NEGATIVE.

- Sets the graph to display positive or negative changes in Absorbance.
  Choose POSITIVE if Absorbance increases with time.
  Choose NEGATIVE if Absorbance decreases with time.

RANGE: Set a number in the range 0 to 3A.

- This sets the graph y-axis. Enter a number slightly larger than the change in Absorbance expected.

FACTOR: Enter the factor for Activity as a number in the range 0.001 to 9999.999.

UNITS: Enters the units of Activity using the TEXT ENTRY page.

- Enters the required description or units of Activity up to 11 alphanumeric characters.

LAMP CHANGE: Select from 315, 320, 325, 330, 335, 340, D2, W, Hg.

- Selects the wavelength at which the source is changed between the Tungsten and Deuterium lamps. Selecting D2, W or Hg overrides any changeover and the selected lamp will be used regardless of the wavelength set.

THE MERCURY LAMP MUST BE SWITCHED OFF WHENEVER IT IS NOT IN USE

OPERATOR: Switches to the TEXT ENTRY screen.

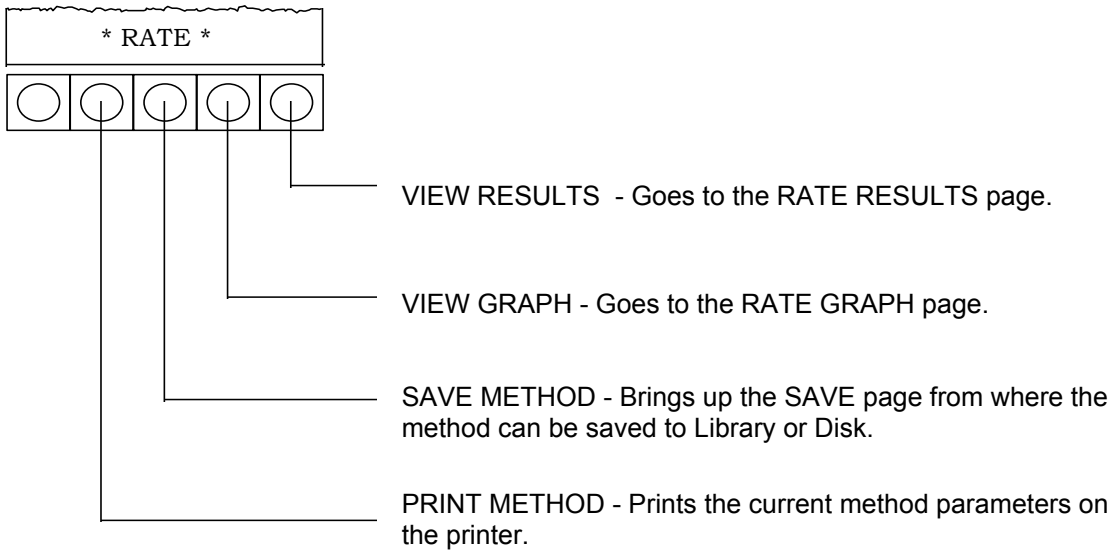
- The operator name is automatically saved with the method and any data produced by the method.

Changing the operator name will not cause the current data to be lost.
If User Log-on is in operation, the operator name cannot be changed.

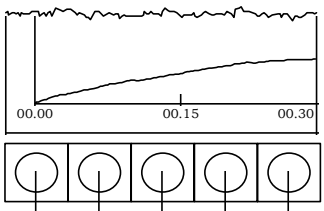
CELL PROG: Switches to the CELL PROG. screen (if fitted).

REF MODE: Toggles the status of the Cell Programmer reference mode (if fitted).

RATE PARAMETERS Page function keys



RATE GRAPH Page



- This page displays the RATE curve and allows it to be manipulated.

VIEW RESULTS - Switches to the RATE RESULTS page.

RATE PAGE - Returns to the RATE PARAMETERS page.

SAVE DATA - Brings up the SAVE screen from where method and data can be saved to disk.

PRINT - Provides a hardcopy of the results i.e. RATE GRAPH and RATE RESULTS. (If a Cell Programmer is fitted see the note below).

MANIPULATE - Brings up the Manipulate options.

- If more than one rate has been run in parallel using the Cell Programmer then three further print options are available: ALL OVERLAY, ALL SEQUENTIAL, and ONE RESULT.

ALL OVERLAY	Prints the results of all cells in the run on one sheet of paper up to a maximum of 4 results. If more than four results are present then the remainder are printed on a second sheet.
ALL SEQUENTIAL	Prints each result in the run on a separate sheet of paper.
ONE RESULT	Prints the result currently displayed.

- Pressing RUN starts a measurement using the current method.
- Pressing ZERO/BASE zeros the instrument using the wavelength specified in the current method. (See page 4).

MANIPULATE

MANIPULATE
TRACK **SECTION** **RESCALE** **SMOOTHING** **ABS DISPLAY** **ORIGINAL** **ANOTHER CELL**

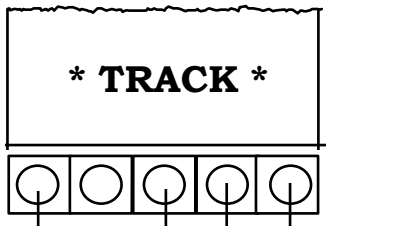
TRACK	Sets the start and stop time for the rate calculations.
SECTION	Sets sequential start and stop times to enable rates to be calculated on up to four sections of the rate curve.
RESCALE	Changes y-axis scale automatically or manually.
SMOOTHING	Allows three levels of smoothing to be applied to the Rate Curve.
ABS DISPLAY	Sets the display of absolute absorbance values or absorbances relative to the first measurement(s) of the run.
ORIGINAL	Resets the graph to display the data as originally collected.
ANOTHER CELL	Only present if the Cell Programmer has been used. Enables the results of another cell from the same run to be displayed.

TRACK

- To move the vertical cursor across the screen use the Left and Right Arrow keys. The cursor always moves to a data point regardless of the displayed scales. Pressing ENTER places a marker at the current time.
- To delete a marker, place the cursor on the marker and press CLEAR.
- The x-axis values are used to recalculate the rate of change of Absorbance between the new start and stop times. Results are listed on the RATE RESULTS page.

Up to four discrete pairs of cursors can be placed on the graph. Arrows are placed on the cursors and results are displayed on the RATE RESULTS page for those parts of the graph indicated by the arrows.

- Selecting SECTION will remove the TRACK markers.
- The minimum interval between TRACK cursors is one second.



VIEW RESULTS - Switches to the RATE RESULTS page.

FAST/SLOW - Toggles between two cursor speeds. In FAST mode the cursor jumps 5% of the graph or to the next data point whichever is the greater. In SLOW mode the cursor jumps to the next data point or the next display pixel whichever is the greater.The function key label shows the next speed ie the opposite to the one selected.

CLEAR ALL - Clears all the markers.

RATE GRAPH - Returns to the RATE GRAPH page.

SECTION

- To move the vertical cursor across the screen use the Left and Right Arrow keys. The cursor always moves to a data point regardless of the displayed scales. Pressing ENTER places a marker at the current time.

- To delete a marker place the cursor on the marker and press CLEAR.

Up to five markers can be placed on the graph. Rate results will be reported between markers providing a maximum of four sets of results (Sections). The minimum Section size is one second.
Results are listed on the RATE RESULTS page.

Selecting TRACK will remove the SECTION markers.

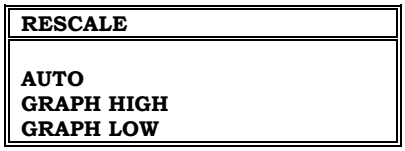
RESCALE

- This option gives a pop-up menu for changing the graph y -axis scale.

- Move the cursor to one of the options and press ENTER to select an operation.

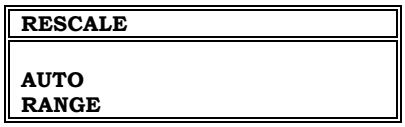
The rescale options depend on whether Absolute or Relative Absorbance has been selected.

Absolute Absorbance:



AUTO	Displays the RATE GRAPH with the y-axis rescaled so that the trace fills the screen.
GRAPH HIGH, GRAPH LOW	Allow the user to set the upper and lower limits for the RATE GRAPH y-axis.

Relative Absorbance:



AUTO	Displays the RATE GRAPH with the y-axis rescaled so that the trace fills the screen.
RANGE	Allows the user to set the upper y-axis value.

ABS DISPLAY

- This option enables the RATE GRAPH to be redisplayed with Absolute Absorbance or Relative Absorbance values.

SMOOTHING

- This option offers a pop-up menu to choose one of three smoothing algorithms. Choices are NONE, LOW, MEDIUM and HIGH. A moving point average is performed on the data and in each case data points will be lost from either end of the data.

SMOOTHING	No of POINTS USED	POINTS LOST AT EACH END
NONE	0	0
LOW	9	4
MEDIUM	17	8
HIGH	37	18

ORIGINAL

This removes any manipulation and displays the rate graph as originally specified by the rate method.

ANOTHER CELL

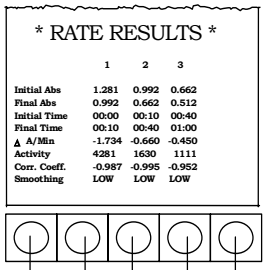
- If more than one rate has been run in parallel using the Cell Programmer then this function allows the results from any cell in the run to be selected and displayed. Enter the number of cells you wish to display.

RATE RESULTS Page

- The Rate Results page displays the Initial and Final Absorbance, Initial and Final Time, the change in absorbance per minute, calculated Activity, Correlation Coefficient of the best fit line and finally the smoothing parameter used.

If the rate curve has been tracked the Initial and Final Absorbance with the Initial and Final Time will reflect those chosen by the two cursors.

Shown below is the Rate Results page after choosing 'SECTION' and the three sets of data represent results calculated for each section. A similar display will be seen with TRACK**.**



VIEW GRAPH - Returns to the RATE GRAPH page.

RATE PAGE - Returns to the RATE PARAMETERS page.

SAVE DATA - Brings up the SAVE screen from where method and data can be saved to disk.

PRINT - Provides a hardcopy of the results i.e. RATE GRAPH and RATE RESULTS.

LIMS EXPORT – Sends the results via the RS232 port.

Parallel Rate Measurements using the Cell Programmer

- The 8 Cell Programmer can be used in conjunction with the RATE software to measure between 2 and 8 cells in parallel.
- For the Cell Programmer to be used it must be ON with MODE set to AUTO.
- The RATE METHOD setup and MANIPULATE functions are exactly the same except that the MEASURE TIME now sets the time between each cycle, i.e. the length of time between measurements on the first cell. The number of measurements taken on each cell is set by the CELL CYCLES parameter on the cell programmer page. The total time over which the measurements are made is the result of the time between measurements (MEASURE TIME) and the number of measurements (CELL CYCLES). For example an analysis using 4 cells with MEASURE TIME set to 15 seconds and CELL CYCLES set to 20 would give a total measurement time of 5 minutes.

To set up a parallel rate method do the following:

- Set up the method as normal on the RATE PARAMETERS page.

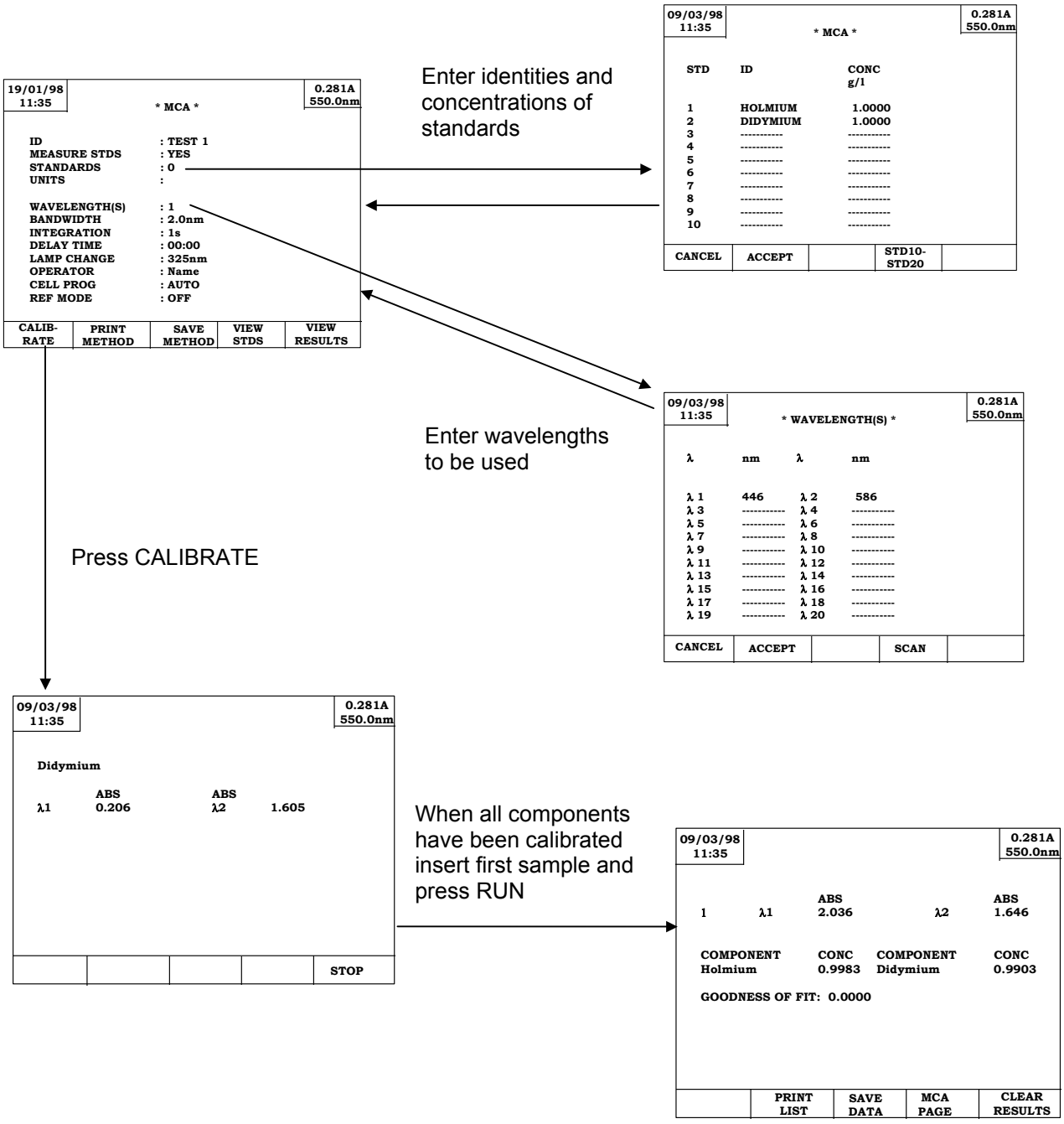
Note that MEASURE TIME specifies the time between each measurement on the first cell.

- Go to the Cell Programmer page. Press HOME then ACCESSORIES and select CELL PROG.
- Set up the cell programmer method as required.
- Return to the RATE PARAMETERS page, press ZERO/BASE to zero the instrument (if required) then press RUN.
- The analysis will proceed with the rate graph for the first cell being drawn on screen.
- To view the result of any other cell press MANIPULATE on the RATE GRAPH page and select ANOTHER CELL. The cell number currently displayed is shown to the right of the ID: line.
- To print the results press PRINT on either the RATE GRAPH page or the RATE RESULTS page.

Three further print options are available: ALL OVERLAY, ALL SEQUENTIAL, and ONE RESULT.

ALL OVERLAY	Prints the results of all cells in the run together in batches of 4. TRACK and SECTION markers are not included.
ALL SEQUENTIAL	Prints each result in the run separately. TRACK and SECTION markers are included.
ONE RESULT	Prints the result currently displayed. TRACK and SECTION markers are included.

MCA


19/01/98 11:35
0.281A 550.0nm
* MCA *
ID : TEST 1
MEASURE STDS : YES
STANDARDS : 0
UNITS :
WAVELENGTH(S) : 1
BANDWIDTH : 2.0nm
INTEGRATION : 1s
DELAY TIME : 00:00
LAMP CHANGE : 325nm
OPERATOR : Name
CELL PROG : AUTO
REF MODE : OFF
CALIB-RATE
PRINT METHOD
SAVE METHOD
VIEW STDS
VIEW RESULTS
Enter identities and concentrations of standards
09/03/98 11:35
0.281A 550.0nm
* MCA *
STD ID CONC g/1
1 HOLMIUM 1.0000
2 DIDYMIUM 1.0000
3 ----------
4 ----------
5 ----------
6 ----------
7 ----------
8 ----------
9 ----------
10 ----------
CANCEL
ACCEPT
STD10-STD20
Enter wavelengths to be used
09/03/98 11:35
0.281A 550.0nm
* WAVELENGTH(S) *
λ nm λ nm
λ 1 446 λ 2 586
λ 3 ---------- λ 4 ----------
λ 5 ---------- λ 6 ----------
λ 7 ---------- λ 8 ----------
λ 9 ---------- λ 10 ----------
λ 11 ---------- λ 12 ----------
λ 13 ---------- λ 14 ----------
λ 15 ---------- λ 16 ----------
λ 17 ---------- λ 18 ----------
λ 19 ---------- λ 20 ----------
CANCEL
ACCEPT
SCAN
Press CALIBRATE
09/03/98 11:35
0.281A 550.0nm
Didymium
ABS ABS
λ1 0.206 λ2 1.605
STOP
When all components have been calibrated insert first sample and press RUN
09/03/98 11:35
0.281A 550.0nm
ABS ABS
1 λ1 2.036 λ2 1.646
COMPONENT CONC COMPONENT CONC
Holmium 0.9983 Didymium 0.9903
GOODNESS OF FIT: 0.0000
PRINT LIST
SAVE DATA
MCA PAGE
CLEAR RESULTS

- The MCA (Multi Component Analysis) application is able to measure up to 20 components in a mixture, measuring up to 20 wavelengths per sample.

- Standards can be measured at run time or loaded from files obtained using the MULTI λ function of FIXED.

MCA METHOD Page

* MCA *	
ID	**TEST 1**
MEASURE STDS	**YES**
STANDARDS	**0**
UNITS	
WAVELENGTH(S)	**1**
BANDWIDTH	**2.0nm**
INTEGRATION	**1s**
DELAY TIME	**00**
LAMP CHANGE	**325nm**
OPERATOR	**Name**
CELL PROG	**AUTO**
REF MODE	**OFF**

ID: Enter a description using the TEXT ENTRY screen.

- The ID identifies the method and will be saved with the method and any spectra produced by the method.

MEASURE STDS: Use ENTER to toggle between YES and NO.

YES - Standards are measured with the run and all fields remain editable.

NO - Standards are loaded from Library or Disk. The Wavelength(s), Bandwidth, Integration, Delay time, Lamp change and Operator Name are also loaded with the standards and cannot be edited. Any attempt to do so causes the prompt “Change method by loading MCA standards” to appear and no action is taken.

Changing the MEASURE STANDARDS parameter will cause all previous data to be lost.

STANDARDS: Switches to the STANDARDS ENTRY screen.

- Identifications and concentrations of up to 20 standards may be entered.

UNITS : Switches to the TEXT ENTRY screen.

- Enter the units for the concentration.

WAVELENGTH(S): Switches to the WAVELENGTH ENTRY screen

WAVELENGTH: The available wavelength range is 190.0nm to 900.0nm

If the wavelength requires the Deuterium lamp then this will be switched on. The current data will be lost if the wavelength is changed.

BANDWIDTH: Select from 4, 2, 1.5, 1, 0.5 and 0.2nm

INTEGRATION: Enter integration time in seconds.

- This sets the integration time for which the result is measured. The minimum is 1s, and the maximum is 9999s.

The current data will be lost if the integration time is changed.

DELAY TIME: Set a time in the range 00.00 to 99.59, using . to separate minutes and seconds. The number of seconds must always be entered explicitly.

- This sets the time between pressing RUN and the start of the measurement. The range is from 0 to 99 minutes and 59 seconds.This field is only available if UVCalc has been installed.

LAMP CHANGE: Select from 315, 320, 325, 330, 335, 340, D2, W, Hg.

- Selects the wavelength at which the source is changed between the Tungsten and Deuterium lamps. Selecting D2, W or Hg overrides any changeover and the selected lamp will be used regardless of the wavelength set.

THE MERCURY LAMP MUST BE SWITCHED OFF WHENEVER IT IS NOT IN USE
The current data will be lost if the lamp change parameters are changed.

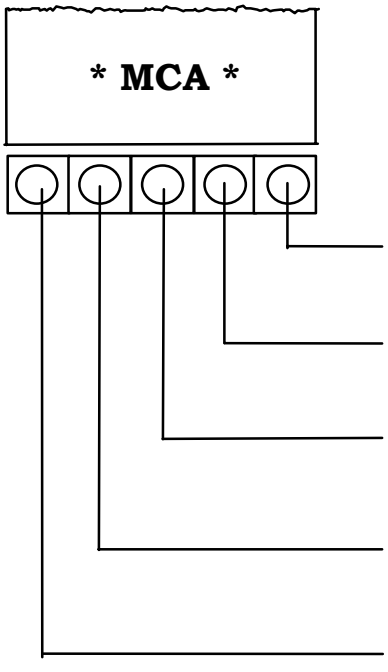
OPERATOR: Switches to the TEXT ENTRY screen.

- The operator name is automatically saved with the method and any data produced by the method.

Changing the operator name will not cause any current data to be lost.
If User Log-on is in operation, the operator name cannot be changed.

CELL PROG: Switches to the CELL PROG. screen (if fitted).

REF MODE: Toggles the status of the Cell Programmer Reference Mode (if fitted).



VIEW RESULTS - Transfers to the Results Table if it contains results.

VIEW STDS - Transfers to Standards results table if a calibration has been performed.

SAVE METHOD - Brings up the SAVE page from where the method can be saved to Disk.

PRINT METHOD - Prints the current method parameters on the printer.

CALIBRATE - Moves to the CALIBRATION PAGE to perform a calibration if standards and wavelengths have been entered.

STANDARDS ENTRY Page

- When MEASURE STDS = YES

  Use the up and down arrow keys to move up and down the list. When the highlight is on the field to be entered or edited press ENTER to display the Text Entry dialogue box. Enter the name of the Standard and press the ACCEPT function key when finished. The instrument returns to the STANDARDS ENTRY page with the concentration field for the standard highlighted. Press ENTER to display the edit dialogue box, enter the concentration using the numeric keypad, and press ENTER when finished. The instrument returns to the STANDARDS ENTRY page with the ID for the next standard highlighted.

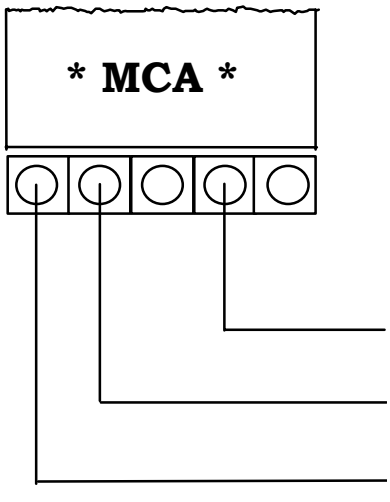
  Up to 20 standards can be entered in this way. The standards are displayed on two pages. The STD11 - STD20 function key toggles between the two pages.

- When MEASURE STDS = NO

  Press ENTER to display the LIBRARY page. Select and load the files for each standard in turn.

  A library of standards can be built up using the MULTI λ function in FIXED. The same method must be used for each MULTI λ result, and will be used for the MCA analysis.When the first MULTI λ file is loaded the current MCA method is changed to that used to obtain the MULTI λ result.

  Standards can thus be used in any combination without having to recalibrate for each new mixture.



STD1 - STD10/STD11 - STD20 - Toggles between displaying the first and second halves of the Standards List.

ACCEPT - transfers to the MCA METHODS page with the new list accepted.

CANCEL - Transfers to the MCA METHODS page leaving the old list unchanged.

WAVELENGTH ENTRY page

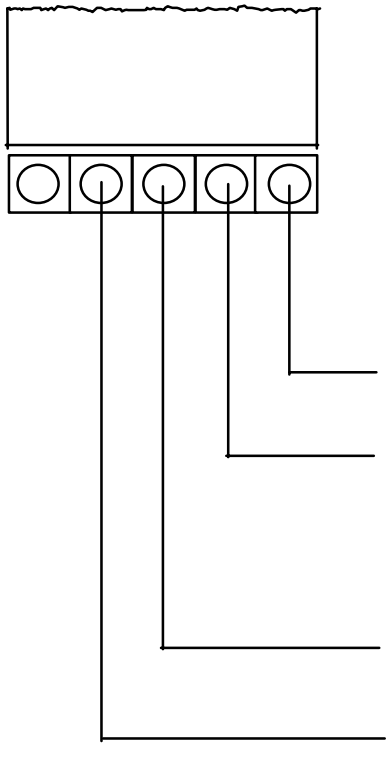
Use the up and down arrow arrow keys to move up and down the list. When the highlight is on the field to be entered or edited press ENTER to display the EDIT box and enter the values with the numeric keys. It is not necessary to enter the values in numerical order, although analysis will be quicker if they are. Press ENTER when finished. The instrument will return to the WAVELENGTH ENTRY page with the new value inserted in the list and the highlight moved to the next wavelength. When all wavelengths have been entered press the ACCEPT function key to return to the MCA methods page using the new list or the CANCEL function key to return leaving the old list unchanged.

Alternatively wavelengths may be entered directly from a scan. Clear the beam(s) and press ZERO BASE to perform a baseline scan, then put the sample in the cell holder and press the SCAN GRAPH function key. The instrument performs a scan using the method currently entered in the SCAN PARAMETERS page.

Use left and right arrow keys to move the vertical cursor to a suitable wavelength and press ENTER to mark it. Repeat until all required wavelengths have been marked. Marks can be removed using the CLEAR key, or the CLEAR ALL function key. When all required wavelengths have been marked press the ACCEPT function key to accept the list and return to the MCA Methods page.

Wavelengths can be selected either from a scan of the mixture to be analysed or by performing a scan on each standard in turn and selecting suitable wavelengths. Wavelengths already entered in the table are shown on the Scan Graph.

At least one wavelength must be entered for each standard.



ACCEPT - Transfers to the MCA METHODS page with all marked wavelengths added to the wavelength list.

FAST/SLOW - Toggles between two cursor speeds. In FAST mode the cursor jumps 5% of the graph or to the next data point whichever is the greater. In SLOW mode the cursor jumps to the next data point or the next display pixel whichever is the greater.

CLEAR ALL - Clears all marks.

RESCALE - Rescales the x and y-axes so that the spectrum fills the screen.

Calibration

When the Standard Identifications and concentrations have been entered via the STANDARDS ENTRY page, and the wavelengths have been entered via the WAVELENGTH ENTRY page, the MCA application is ready for calibration.

Clear the beam(s) and press ZERO/BASE to perform a baseline scan.

Press the CALIBRATE function key from the MCA METHODS page. If any results are present you will be given the option to proceed or cancel, with PROCEED highlighted.

All previous data will be lost if PROCEED is selected.

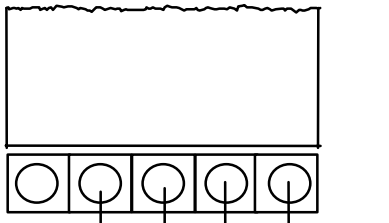
Press ENTER to proceed. The message “Press RUN to measure STD1: “ will be displayed. Put the first standard in the beam then press RUN. Continue until all standards have been measured. Results for each standard will be stored in the Calibration Results Table with results for each standard on a new page. Use the up and down arrow keys to move between standards.

When the last calibration has been done put the first sample to be analysed in the beam and press RUN.

Analysing a Sample

When a calibration has been performed or loaded with the method the MCA application is ready to use.

When RUN is pressed from the METHOD or RESULTS pages the instrument will measure the absorbance of the sample at each of the wavelengths specified in the method and compare with the absorbances of the standards at these wavelengths. The concentrations of each component are calculated and displayed on the results page. Results for each sample are displayed on a new page. Use the up and down arrow keys to move through the pages of results.



CLEAR RESULTS - Clears the results table.

MCA PAGE - Returns to the MCA METHOD page.

SAVE DATA - Displays the SAVE page from which the results can be saved to Library or Disk.

PRINT LIST - Prints the list on the selected printer

UVCalc

Introduction

Quantitative analytical procedures are built around two fundamental key principles, measurement of the parameter, and subsequent calculations based on these measurements.

In UV-Visible spectrophotometry, and many other ‘mature’ techniques the science associated with the measurement of the parameter is well developed. There are fully validated ‘test kits’ available from the leading chemical suppliers in the key areas of bio-chemical and environmental / water chemistry. In addition, most laboratories also have their own fully developed internal procedures.

With defined procedures, many ‘standard methods’ will document the final calculation in the form of an algebraic formula. *Uvcalc* allows these formulae to be entered in to the software method, together with the control limits, providing automatic calculation of results from measurements using user-defined equations and indication of conformity to the supplied control limits. The measurement is obtained from the spectrophotometer in the form of a reading at a specific wavelength in Scan methods and individual results in Fixed and Quant methods.

This manual should be read in conjunction with the main instrument operating manual and also the *uvcalc-aqua* or *uvcalc-bio* manual where these have also been purchased

Specification

Up to 4 different equations may be applied to each measurement.

The formula editor supports +, -, *, /, and bracketing.

Allowed operands include Measurements, Constants (entered via the numeric keypad), fixed & variable factors (input by the user at run-time) and *uvcalc* results from preceding equations.

Each formula may have up to 20 characters

Each formula will support up to 9 different of each of the measurements, constants , variable factors and results.

Equations will be saved with the current application method, and *uvcalc* results saved with the current results.

Equations, results, units and pass /fail statuses are included on the hardcopy output.

Operation

General Comments

On each of the scan, fixed and quant pages, a new line headed *uvcalc* will appear when the *uvcalc* software is installed. With no equations programmed the field next to *uvcalc* will be 0

Pressing enter when the *uvcalc* line is highlighted will present a list of 4 *uvcalc* equations (empty when first installed).

Highlighting and entering one of these will present the equations parameters page in the following format:

FORMULA:
TITLE:
UNITS:
TEST RESULT: NO
UPPER LIMIT: 0.000
LOWER LIMIT: 0.000

There will also be lines specific to the particular application (scan, fixed or rate - see separate headings)

FORMULA
To enter a formula, select **FORMULA** and press ENTER. A “keyboard” will appear, with the following symbols:

M F R ( )
\+ - * /
SPACE

- **M** Measurement. On selecting this a pop up appears providing the choice between Once only and repeated measurements. (Replaced by λ in “SCAN”)
- **F** Variable factor to be input by the user at run-time.
- **R** *uvcalc* result from preceding equations.

The required formula can then be built up by highlighting the required symbol and pressing “ENTER”

NB: Navigation around the screen is achieved in all cases as per the normal operation of the software, ie. using the arrow keys to move around.

To clear the formula, press “C”. To accept it, press ACCEPT

TITLE & UNITS allow the user to enter a suitable description and units for the equation.

TEST RESULT toggles between “ON” & “OFF”, whilst the “LIMIT” lines set the allowable limits for the test.

Scan

Up to 9 different measurements may be specified for each Scan *uvcalc* equation. These are denoted by 1…9. The wavelengths at which these measurements are made can be specified in one of 2 ways:

They can be entered numerically before the scan

They can be entered after the scan using a peak picking process. This appears as an extra parameter on the equation parameter page (USE TRACKING). The selected wavelengths will then be fed into the method so that the subsequent final result will be calculated automatically.

One-off factors are input by the user before the first scan.

If you subsequently move from the results/graph pages back to the main menu, the one-off factors will be reset and must be entered again before the next run.

Fixed

Up to 9 different measured results may be specified for each *uvcalc* equation. These measurements will comprise a combination of up to 9 different one-off measurements (measured at the start of the run only) and one measurement which will be re-measured with each press of RUN

Quant

Up to 9 different measurements may be specified. These measurements may be either a standard (S1…S6) (measured as part of the normal calibration process) or a sample (X)

One-off factors will be cleared if you select CLEAR RESULTS from the results page or if you return to the main menu.

UVCalc how to

How to set up a Fixed calculation

To set up the application: M1 * 50.0

On the FIXED page, go to the *uvcalc* line and press ENTER

Go to **EQUATION 1** and press ENTER

Go to **FORMULA** and press ENTER

Highlight "**M**" and press ENTER

A pop-up will appear giving the choice of
ONCE ONLY, CONSTANT
MEASURE EACH RUN

Highlight "**MEASURE EACH RUN**" and press ENTER

Highlight "*****" and press ENTER

Key in "50"

Press **ACCEPT**

This will return you to the main uvcalc page

Make appropriate entries for the TITLE and UNITS line

Press **ACCEPT** twice

This will return you to the FIXED page

Insert sample and press RUN

The results page will display the actual absorbance value and also the result of the calculation.

How to set up a Scan application

To set up the application: λ_1/λ_2 * F

On the SCAN page, go to the *uvcalc* line and press ENTER

For this example ensure that **START** = *400 nm and* **STOP** = *600 nm.*

Go to **EQUATION 1** and press ENTER

Go to FORMULA and press ENTER

Highlight "λ" and press ENTER

An edit box will appear.

Key in "450" for the first wavelength and press ENTER.

Highlight "/" and press ENTER

Highlight "λ" and press ENTER

The edit box will again appear.

Key in "500" and press ENTER

Highlight "*" and press ENTER

Highlight "F" and press ENTER

A pop-up will appear giving the choice of:
FIXED FACTOR
VARIABLE FACTOR

Highlight "Variable Factor" and press ENTER

Enter a suitable ID, and press ACCEPT

Add suitable Title and Units

Press ACCEPT twice

Press RUN

You will be asked to enter a factor

The instrument will now scan and a results page will appear with the result of the calculation.

How to edit an existing method

How to add parameters to the end of an equation

e.g. to modify M1*50.0 , by adding a weight correction, so the equation becomes **M1*50.0 *(F1/F2)**

Where F1 = Nominal weight (Fixed Factor)
F2 = Actual weight (Variable Factor)

On the FIXED page, go to the *uvcalc* line and press ENTER

Go to **EQUATION 1** and press ENTER

The equation prepared in section 5.1 should be displayed

Go to **FORMULA** and press ENTER

The cursor should be at the end of the existing formula

Highlight "*****" and press ENTER

Highlight "**(** " and press ENTER

Highlight "**F**" and press ENTER

A pop-up will appear giving the choice of
FIXED FACTOR
VARIABLE FACTOR

Highlight "Fixed" and press ENTER

Enter a suitable ID for the factor and press ACCEPT

Highlight "*/*" and press ENTER

Highlight "**F**" and press ENTER

This time, select "Variable Factor" from the pop-up

Enter a suitable ID for the factor and press ACCEPT

Highlight " **)** " and press ENTER

Press **ACCEPT** to return to the main *uvcalc* page.

Press **ACCEPT** twice more to return to the FIXED page

Insert sample and press **RUN**. You will be prompted when to input the factor values.

How to modify an equation

e.g to modify the initial equation to: **(M2-M1)*50.0**

Where M1 becomes a once only constant
and M2 becomes measure with each run

On the FIXED page, go to the *uvcalc* line and press ENTER

Go to **EQUATION 1** and press ENTER

The equation prepared in the example above should be displayed

Go to **FORMULA** and press ENTER

The cursor should be at the end of the existing formula

Press **SWITCH FIELDS** and navigate the cursor to "**M1**". Press ENTER

Alter selection to "**ONCE ONLY**"

Press **SWITCH FIELDS**

Enter the "**(** " , "**M2**", and "**-**" .

For M2 , select "Measure with each run"

Press **SWITCH FIELDS** and move the cursor to the "*****"

Press **SWITCH FIELDS** again and add the closing bracket.

Press **ACCEPT**

This will return you to the main uvcalc page

Make appropriate entries for the TITLE and UNITS line

Press **ACCEPT** twice

This will return you to the FIXED page.

UVCalc error messages

The following error messages may occur if you make a mistake in entering an equation or in setting the system up.

ONLY 1 FACTOR MAY BE ENTERED WITH SAMPLE
You have attempted to create a formula with two or more factors for each sample

THIS FORMULA HAS TOO MANY CONSTANTS
You have created a formula with more than 9 numbers in it.

FORMULA CONTAINS AN INVALID NUMBER
You have attempted to create a formula with an invalid input

BRACES DO NOT MATCH IN FORMULA
You have created a formula with too many brackets at one end

ALL BINARY OPERATIONS REQUIRE TWO OPERANDS
You have created a formula with an incomplete arithmetical operation
(e.g. 3-+4)

INVALID COMBINATION OF OPERANDS
You have created a formula with missing operator(s)
(e.g. F1(M1))

BRACE MISSING?- UNMATCHED CLOSE BRACE
You have created a formula with a close brace(bracket) before or without an open brace.

THIS FORMULA CANNOT START WITH THIS TOKEN
In QUANT mode, you have created a formula with an invalid initial token (i.e. an operator rather than an operand)

FORMULA CONTAINS OUT OF RANGE STANDARD
A specified standard is no longer in the calibration.

ONLY ONE MULTIPLE MEASUREMENT IS ALLOWED
In FIXED mode, you have created a formula with an invalid initial token

FORMULA CONTAINS INVALID RESULT TOKEN
The result from an earlier calculation is no longer being produced.

UVCALC :INVALID CELL PROGRAMMER MODE
An invalid cell programmer mode has been selected. Check settings

FORMULA CONTAINS OUT OF RANGE WAVELENGTH
You have selected wavelengths outside the range set for the scan

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Thermo
ELECTRON CORPORATION

Contents

1. Introduction

This document provides all the essential information required to perform the correct installation to a basic operating level of a Nicolet Evolution 500 spectrophotometer with Local Control software. This is reproduced in the Regulatory environment as Installation Qualification (IQ) and Operation Qualification (OQ) of the specified product.

The Validator 5 Log Book contains full instructions for Installation/Operational Qualification of your Thermo Electron UV-Visible spectrophotometer system. It is available as a purchased option and can be ordered from your local Thermo Electron authorized Sales/Support organization (Part Number 10 03 0101).

This IQ/OQ procedure together with the completed Test Progress Sheet should be removed from this manual and filed for future reference in your Validator 5 Log Book.

Where appropriate, references will be made to the required manual.

1.1 Identification

Nicolet Evolution 500 Series Local Control Software.

1.2 Manufacturer

Thermo Electron Corporation
Mercers Row
Cambridge
CB5 8HY
UK

1.3 General Description

Nicolet Evolution 500 spectrophotometers have been designed for analytical applications in which fast, accurate and reproducible spectrophotometric measurements are required. The Local Control software provides control of the spectrophotometer via the use of the integral keypad and liquid crystal display.

1.4 Compliance Features

Features designed to assist the laboratory in recording and providing documentation for compliance include the following:

- User log-on and access control.
- All data is tagged with a unique system identifier which includes instrument type and serial number, software version number etc.
- All data is date & time stamped.
- All analytical calibrations are stored with the data file.
- In-built calculations (optional) using ***uv****calc* software.

2. Product History

Since its initial release, the Local Control software has been updated at specified intervals to provide additional functionality, both in terms of software capability and accessory control, and to implement corrective actions. Each successive release is identified by a unique version number, displayed on the liquid crystal screen.

2.1 Development/Release History

Nicolet Evolution 500 Local Control software is a development of Thermo Electron's well-established UV-Visible Local Control Software; while building on the firm foundation of its predecessor it also incorporates significant enhancements.

Local Control Software has a well-demonstrated history of problem-free usage in the laboratory. Customer experience has demonstrated consistent conformance to software and system requirements. When used as specified, there have been no reports of safety problems.

Version 1.00 – 25 July 1993	Initial release of the software.
Version 2.00 – 20 October 1993	Rate functionality added. Service release.
Version 2.02 – 16 November 1993	Higher Order derivative functionality added to Scan.
Version 2.04 – 3 December 1993	Service release.
Version 3.00 – 4 February 1994	Support for UV3 and UV4 added. Service release.
Version 3.10 – 23 February 1994	French and Spanish languages added.
Version 3.31 – 25 March 1994	German language added.
Version 3.32 – 20 April 1994	Service release.
Version 3.50 – 31 August 1994	Support for Gilson XL Autosamplers added. Service release.
Version 3.51 – 25 October 1994	Service release.
Version 4.00 – 22 March 1995	Service release.
Version 4.11 – 15 November 1995	Service release.
Version 4.15 – 28 February 1996	Service release.
Version 4.21 – 6 June 1997	Service release.
Version 4.24 – 9 September 1997	UVCalc advanced results calculation added. Service release.
Version 4.30 – 10 November 1997	Support for new printers added.
Version 5.00 – 21 April 1998	Support for UV300/500. Internal mercury lamp support, enhancements to Quant/Serial/Fixed/MCA analyses.
Version 5.01 – 29 April 1998	Service release.
Version 5.02 – 6 May 1998	Service release.
Version 5.03 – 19 May 1998	Service release.
Version 5.04 – 20 May 1998	Service release.
Version 5.05 – 5 August 1998	Service release.
Version 5.06 – 23 December 1998	Correction of Action Requests received since the release of V4.20.
Version 6.04 – 24 December 1999	Service release.
Version 6.06 – 11 January 2000	Service release.
Version 6.07 – 18 January 2000	Service release.
Version 6.51 – 4 December 2000	Service release.
Version 6.53 – 7 December 2000	Service release.
Version 5.56 – 17 September 2001	Service release. Modifications to user log-on.
Version 7.00 – 23 July 2003	Support for Evolution 500. Correction of Action Requests received since the release of V6.56.

NOTE: WHILST EVERY EFFORT IS MADE TO ENSURE THAT THIS RELEASE HISTORY IS CURRENT, THERE WILL BE TIMES WHEN CHRONOLOGICALLY THIS LIST MAY NOT REFLECT THE LATEST RELEASE(S) OF SOFTWARE. IN THESE CIRCUMSTANCES AN AMMENDMENT TO THIS TEXT WILL BE AVAILABLE ON REQUEST.

3. Technical Description

The Local Control software provides control of the spectrophotometer via the use of keypad and liquid crystal display.

Under the five identified applications of Scan, Fixed, Quant, Rate and MCA it provides the functionality of wavelength scanning, single fixed wavelength measurement, quantitation using a calibration graph constructed from standards of known concentration, and absorbance vs time measurements. Mass data storage is provided by an instrument memory library, or by writing to

a PC compatible disk. In addition to this basic functionality, there are control functions for spectrophotometer set-up, accessories, performance qualification, customized calculations etc.

3.1 Thermo Electron Accessories Directly Supported

- Calibration Validation Unit (CVU)
- SuperSipper
- 8-Cell Changer

3.2 Product Documentation

Nicolet Evolution 500 User Manual

3.3 Product Development & Evaluation

This product has been developed and evaluated according to the procedures placed on the Thermo Electron Corporation by the ISO 9001 registration.

3.4 Qualification/User Installation

The processes detailed below form an essential part of any System Validation. These documents and their structure are based on the requirements of the UK Pharmaceutical Industry Computer Systems Validation Forum (PICSVF). These guidelines were published in their document "Pharmaceutical Industry Supplier Guidance - Validation of Automated Systems in Pharmaceutical Manufacture", later formally adopted as the GAMP Guidelines.

4. System Acceptance Test Specification

4.1 Introduction

Author: Dr Craig Fellows **Version Number:** 5

Title: Product Manager

This document describes the tests required for the specific Installation Qualification (IQ) and Operational Qualification (OQ) of the Nicolet Evolution 500 Local Control Software and references appropriate sections of the user documentation.

4.2 Scope

This test specification details the Qualification procedures required for:

Initial Power Up

System Initialization

System Functionality

Data Save and Transfer

Spectrophotometer Compliance to Specification

4.3 Overview and Test Plan Section

Section 4.5 describes in detail the tests required for this procedure. Each test has its own unique identifier.

Results should be recorded on the Test Progress Sheet supplied with this plan. If the result of the test is a pass the ‘Pass’ should be circled. If the result is a failure the ‘Fail’

should be circled. If a test is hardware or software specific and is not present the 'N/A' should be entered, N/A meaning Not Applicable.

In the event of a test failure and corrective action taken, this should be reported on a copy of the Test Incident Sheet, a master of which is supplied in the Template Masters section of the Validator Log Book.

Testing will require the presence of two persons - one to perform the test the other to act as a witness.

This requirement can be effectively met by having this validation process completed by a trained Thermo Electron authorized Customer Support Engineer, witnessed by the Customer. Contact your local Thermo Electron authorized Sales/Support organization should you wish use this option.

4.4 Testing Requirements

To perform this System Acceptance Test the following must be available:

- Nicolet Evolution 500 User Manual.
- A 3.5 inch floppy disk and a PC with Windows are required to verify data export.
- UVM 001 - Analytical Procedures for a UV-Visible spectrophotometer.
- Calibration Validation Carousel (CVC) or other suitable CRMs for checking the fundamental specification parameters e.g. wavelength, absorbance, etc., as detailed in UVM 001.
- Suitable samples, or filters, for analysis.

4.5 Test Procedures

4.5.1 PP1 - Initial Power Up

Apply power to the spectrophotometer. Do not apply power to any connected PC.

After a pause of approximately 1 minute the LCD display should show the Initialization page.

The information at the top of the screen should display a valid date and time, instrument type and serial number, and will clearly vary from system to system.

Appearance of this page constitutes a pass to this test.

Note: Should the display 'light-up' but no 'picture' appear, check the LCD contrast. LCD display contrast can be controlled using a contrast wheel under the left side of the instrument.

4.5.2 PP2 - System Initialization

The spectrophotometer should now begin to initialize with a √ pass mark appearing alongside each test as it is completed. The Initialization page will automatically then switch to the Home page.

Appearance of the page detailed above constitutes a pass to this test.

4.5.3 PP3 - System Functionality - Setup

1. Ensure the Local Control Screen is on the Home page (if not press the Home key).

2. Press SETUP, use the up/down arrow keys to select Clock, press Enter. Select Hours, press Enter.
3. Change the number to indicate the correct hours. Press Enter.
4. Select Minutes, press Enter.
5. Change the number to indicate the correct minutes. Press Enter.
6. Select Day, press Enter.
7. Change the number to indicate the correct day. Press Enter.
8. Select Month, press Enter.
9. Change the number to indicate the correct month. Press Enter.
10. Select Year, press Enter.
11. Change the number to indicate the correct year. Press Enter I Accept.
12. Press Home.

Problem free operation of these processes and the display of the correct date and time constitute a pass to this test.

4.5.4 PP4 - System Functionality - Scan

1. Ensure that the Application is set to Scan (if not press Home I Scan I Enter).
2. Set the scan type to standard, the scan speed to 600 nm/min, the data interval to 1 nm, the start wavelength to 435 nm and the stop wavelength to 475 nm. Other wavelengths may be selected if a filter other than a holmium filter is used.
3. Place a holmium filter, or other suitable filter, in the sample position.
4. Press the Run button.

The appearance of a new spectrum on the display constitutes a pass to this test.

4.5.5 PP5 - System Functionality - Data Store and Library

1. Ensure that the Application is set to Scan (if not press Home I Scan I Enter).
2. Save the data produced from the PP4 System Functionality procedure. (Press Save Data, enter the file name PP5 (or another suitable file name), Press Accept I Save).
3. Check that the Data has been stored (Home I Library I Enter).
4. Re-enter the Scan application (Press Home I Scan I Enter).
5. Scan a new sample using the same conditions as PP4. This should be a different sample to that used for PP4.
6. Recall the data produced in PP4. (Press Home I Library I Enter I PP5 (or the file name used) I Enter I Load I Enter).
7. The saved spectrum should be visible on the display.

The successful completion of these tasks constitutes a pass to this test.

4.5.6 PP6 - Data Transfer to Other Packages

1. Ensure the Application is set to Scan (if not press Home I Scan I Enter).
2. Export the data produced from PP4 System Functionality procedure. (Press Save Data, enter PP5 (or another suitable name) for the filename, change the file type to CSV, ensure the Drive is set to Disk, place a floppy disk in the disk drive and press Save).
3. Using a PC, open Windows NotePad and load the .csv file. (Another program that will load .csv file types may be used).

The successful loading of data into NotePad (or another program that can load .csv file types) constitutes a pass to this test.

4.5.7 PP7 - System Functionality - Fixed

1. Ensure the Application is set to Fixed (if not press Home I Fixed I Enter).
2. Press the Run button.

New data in the Results screen constitutes a pass to this test.

4.5.8 PP8 - System Functionality - Quantitation

1. Ensure the Application is set to Quant (if not press Home I Quant I Enter).
2. Select Standards and press Enter. Enter the values for 4 standards and press Accept. (Any standards may be used but the absorbance values should be about 0.5, 1.0, 1.5 and 2.0 A).
3. Zero the spectrophotometer (Press ZeroBase).
4. Calibrate the method (Press Calibrate and follow any prompts).
5. Place a sample, with an expected absorbance between 0.5 and 1.5, in the sample position.
6. Press the Run button and follow any prompts.

New data on the Results screen and a calibration curve in the Quant Graph screen constitute a pass to this test.

4.5.9 PP9 - System Functionality - Rate

1. Ensure the Application is set to rate (if not press Home I Rate I Enter).
2. Press the run button and follow any prompts.

A graphical display of absorbance against time on the Rate Graph screen constitutes a pass to this test.

4.5.10 PP10 - System Functionality - Multicomponent Analysis

This test requires a holmium filter and a didymium filter. If only one wavelength filter is available, a 1 A filter may be used in place of the second wavelength filter.

1. Ensure the Application is set to Multicomponent Analysis (if not press Home I MCA I Enter).
2. Set up an MCA method as follows:
   Ensure that Measure Standards is set to Yes (if not, highlight and press Enter).
   Highlight Standards and press Enter. Set up the Standards Table as follows:
   Standard 1 ID = HO, Concentration = 2
   Standard 2 ID = DY, Concentration = 6
   Press Accept. Highlight Wavelengths and press Enter.
   Enter the following wavelengths: 446, 454, 530, and 586 nm. Press Accept to return to the MCA Method page.
3. Press the Calibrate function key.
   When prompted for the first standard put the holmium filter in the sample beam and press Run.
   When prompted for the second standard put the didymium filter in the sample beam and press Run.
   This completes the calibration.
4. Now run a sample.
   Put the Holmium filter in the sample beam and press Run.

Completion of the measurements and calculation of concentration values constitute a pass to this test.

4.5.11 PP11 - System Functionality - UVCalc Bio

1. Load the method CELLGROW.FXD from the UVCalc Bio floppy disk. (Home I Library I View Disk I CELLGROW.FXD I Enter I Load I Enter).
2. Press Run.

New data on the Fixed Results Screen constitutes a pass to this test.

4.5.12 PP12 - System Functionality - Access Control

1. Ensure the Local Control Screen is on the Home page (if not press the Home key).
2. Press Setup I Environment I User Log-on I Enter.
3. Enter ADMIN and press Accept.
4. Press Change Users.
5. Add a new user called TEST (move the cursor to an empty field and press Enter, enter the Name TEST and press Accept).
6. Add the password TEST for the new user TEST (press Enter, enter the password TEST and press Accept).
7. Press Accept I Home I Log Off I Proceed I Enter.
8. Verify a choice of users is now displayed.
9. Select ADMIN, press Enter, type the password ADMIN, press Accept.
10. Press Setup I Environment I User Log-on I Enter.

The successful completion of these tasks constitutes a pass to this test.

4.5.13 PP13 - System Operational Qualification - Spectrophotometer Compliance to Specification

Check the fundamental instrument parameters of Wavelength Accuracy, Absorbance Accuracy, Stray Light, and Drift. Only a pass in all of these parameters constitutes a pass to this test.

These procedures are best performed using a Thermo Electron Calibration Verification accessory – a Calibration Validation Unit (CVU). Other suitable Certified Reference Materials (CRMs) may be used for checking the fundamental specification parameters or any of the tests specified in UVM 001 (Located in the Validator 5 Log Book) can be used as an alternative.

4.6 Glossary

Installation Qualification (IQ)

Installation Qualification involves the checking of equipment and control system(s) against the supplier standards of operating environment, physical connection, safety parameters and functional parameters prior to the initial utilization of the system. In other words confirming that the system is properly installed.

Operational Qualification (OQ)

Operational Qualification is the process of demonstrating that the equipment will perform consistently as specified over all intended ranges.

CVU –Calibration Validation Unit

CVU (NPL) - Nicolet Evolution 500
CVU (NIST) - Nicolet Evolution 500

Certified Reference Material (CRM), certified traceable to International Primary Reference Materials, by an ISO/IEC accredited process.

4.7 Approved Report Formats for System Acceptance Tests

The following pages of the plan supply the plan Test Progress Sheet(s) for the documented tests.

TEST PROGRESS SHEET 1 OF 2

System: *Customer generated number for the complete system is entered on the spine of the Validator Log Book.*							
Test Ref	***Run Number***	***1***	***Tester Initials***	***2***	***Tester Initials***	***3***	***Tester Initials***
PP1	***Date:*** ***Result:***	***Pass*** ***Fail***		***Pass*** ***Fail***		***Pass*** ***Fail***	
PP2	***Date:*** ***Result:***	***Pass*** ***Fail***		***Pass*** ***Fail***		***Pass*** ***Fail***	
PP3	***Date:*** ***Result:***	***Pass*** ***Fail***		***Pass*** ***Fail***		***Pass*** ***Fail***	
PP4	***Date:*** ***Result:***	***Pass*** ***Fail***		***Pass*** ***Fail***		***Pass*** ***Fail***	
PP5	***Date:*** ***Result:***	***Pass*** ***Fail***		***Pass*** ***Fail***		***Pass*** ***Fail***	
PP6	***Date:*** ***Result:***	***Pass*** ***Fail***		***Pass*** ***Fail***		***Pass*** ***Fail***	
Tester Signature: ***Print Name:***					***Tester Initials*** ***DATE*** *(check customer format)*		
Witness Signature: *(Sign only if this page is completed)* ***Print Name:***					***DATE:***		

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TEST PROGRESS SHEET 2 OF 2

Test Ref	Run Number	1	Tester Initials	2	Tester Initials	3	Tester Initials
PP7	Date: Result:	Pass Fail		Pass Fail		Pass Fail	
PP8	Date: Result:	Pass Fail		Pass Fail		Pass Fail	
PP9	Date: Result:	Pass Fail		Pass Fail		Pass Fail	
PP10	Date: Result:	Pass Fail		Pass Fail		Pass Fail	
PP11	Date: Result:	Pass Fail N/A		Pass Fail N/A		Pass Fail N/A	
PP12	Date: Result:	Pass Fail		Pass Fail		Pass Fail	
PP13	Date: Result:	Pass Fail		Pass Fail		Pass Fail	
Tester Signature: Print Name:				Tester Initials DATE (check customer format)			
Witness Signature: (Sign only if this page is completed) Print Name:				DATE:			

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