PIKE TECHNOLOGIES
Spectroscopic Creativity

Installation and User Guide

AutoPRO Software
Version 5.1

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Introduction

Welcome to AutoPRO, a Windows based accessory automation software program for use with PIKE automated accessories and the PIKE AutoPRO motion controller. With this software package a range of automated accessories may be programmed and operated in conjunction with most Windows based FTIR software packages.

The main program in this software package is **AutoPRO Control**, which contains the tools required to program, operate and perform data collection using your automated accessory. The program is designed for use in conjunction with your FTIR software package, extending and enhancing your analysis needs, and enabling completely automated, unattended operation. The user interface design of AutoPRO is such that the most common operations are accessed with the minimum number of mouse clicks, allowing you to access all portions of the software functionality in the simplest, most convenient manner.

Provided with your software are example profile files for all PIKE Automated accessories. You may wish to use these sample files as you learn about the software. Also provided are example macros for most manufacturers' FTIR packages. Using these macro examples, you will be able to customize your software to perform dedicated analyses.

Security is provided, so that a system administrator is able to set up a complete dedicated analysis. All data collection, storage and manipulation parameters may be "locked down".

Figure1: Front Cover of the AutoPRO CD

Unpacking Your Software

In order for you to quickly verify receipt of your accessory, we have included a packing list. Please inspect the contents of the shipping box carefully. Contact PIKE Technologies immediately if any discrepancies are found.

Packing List

AutoPRO Manual
PN 350-000070-02
Quantity 1

AutoPRO CD
PN 007-040000
Quantity 1

Inside This Manual

This manual contains three major parts. The introduction describes how to install the software, use custom configurations, and security features. The main body of the manual describes the use of the software provided, describing each function in detail.

The final part of the manual describes how to run dedicated applications, and includes sample macros for you to use.

AutoPRO is a Microsoft Windows compliant program. The program was designed to run within Windows 9x, 2000, XP and Windows 7. It is recommended for Pentium based computers with EGA or VGA monitors. A Microsoft compatible mouse is required to access all of AutoPRO's features.

Installing the Software

Step 1: Insert the CD into the drive of your computer.

Step 2: From the START menu, select **Run**. The **Run** dialog box will appear to enter a filename.

Enter either: **X:setup.exe** or "browse" to the Disk Directory and select **setup.exe**.

A setup dialog box will appear for a few moments while the installation program checks for available memory and configuration.

The AutoPRO Setup dialog box will appear:

Choose to use the default path select	Enter
OR	
Choose to enter an alternative path and then select	Enter
OR	
Choose to exit Setup by selecting	EXIT

The software will be copied. The source and destination files and percentage of completed task are displayed.

A dialog box will appear when the program has been loaded. Click on the OK box to complete the installation.

Starting AutoPRO

There are several ways in which to run AutoPRO control. Follow the steps below in order to start AutoPRO Control as a stand-alone application:

1. Click the start button

2. Point to Programs

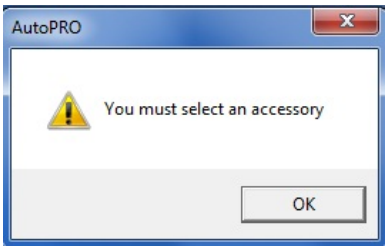
3. Point to the AutoPRO5 folder

4. Click on the AutoPRO program

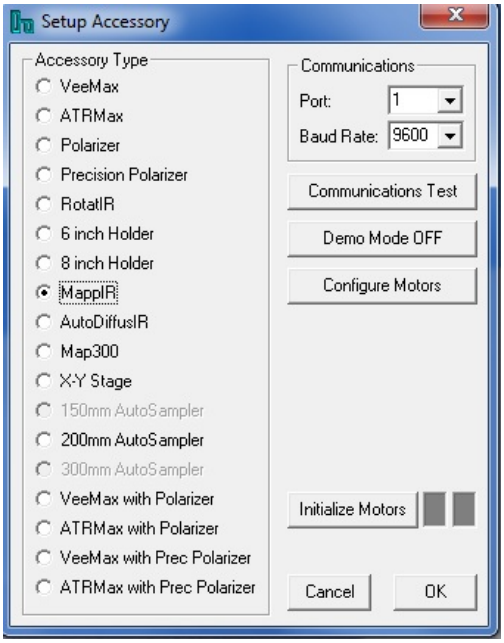
The program will be run, and will be displayed in the lower left hand corner of the display. Note that AutoPRO requires that your computer system be set up with a screen resolution of at least 800x600.

It's Your First Time

When you start AutoPRO for the first time, the software does not know which accessory you have and you will be asked to configure the software. The dialog below will be shown.



When you click OK, the Accessory Setup page will be displayed.



In order to configure the software to work with your accessory, click the button next to the accessory description.

It is now a good time to set up your communications so that you are able to send commands to the motor controller to move your accessory.

Configure Communications

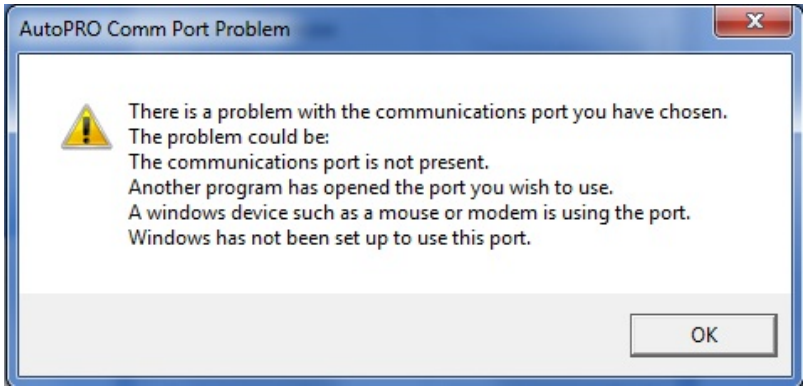
There are two settings that are required to configure communications. These are the Baud Rate and the Communications Port you wish to use.

Baud Rate

9600 baud needs to be used. If you experience communications problems, or are using a slower computer, you may need to select a different RS232 communications port.

Communications Port

There is a choice of four ports that may be selected. Most PC's are equipped with two ports, Com1 and Com2. If you select a port that is not available on your computer such as Com1 when Com1 is not actually present, the following error box will appear.



There are several reasons why this error message may appear:

1. **Windows has not been set up to use a com port.**
   You may check for this by clicking on ports in the Windows Control Panel. The ports that are present are shown. Click on the port you wish to use to view their properties.

2. **The port is in use by another program.**
   If you are already running a program that uses a communications port when you first run AutoPRO, the communications port that the first program is using will not be available to AutoPRO.

3. **The port is assigned to a modem.**
   The port may be assigned to a modem. This assignation is usually done in the config.sys, autoexec.bat file or Windows configuration files and is completed after first entering Windows. If this is the case, use another port.

Communications Test

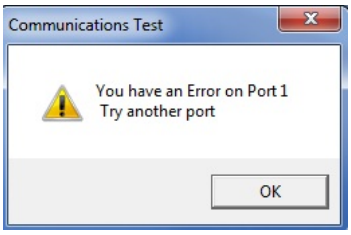
Some computers that are sold today have two serial port connectors on the rear of the computer. However, in some cases, one of these connectors may not be internally connected. For instance, if an internal modem is fitted, this modem may be dedicated to Com2. If you have a problem establishing communications, a loopback connector is supplied with your accessory. This connector connects the transmit line to the receive line of the communications connector on your PC. To use this connector:

1. Plug the connector into the Com port that you wish to use.

2. Select the Com port in the software from the list provided.

3. Click on the **Communications Test** Button, and the following box appears.

4. Click on the **Check Port** button. The software will first test to see if the port is present. If the port is not present, the error message shown below will appear. If the port is present, the software configures the port and sends a message out on the transmit line of the port. Since the loopback connector connects the transmit and receive lines of the communications port, this test message should appear on the receive line. If the software does not receive this message, the following error is displayed.



If you see this message, the communications port that you wish to use is not internally connected. You must review the User manual that came with your computer, or try another port.

If the test is successful, the following message will appear.

You have now successfully established a communications link between your computer and the AutoPRO motion controller. The next time the software is run it will default to this new configuration.

NOTE: Remember to remove the loopback connector after completing this test and reinstall the RS232 cable!

Now that you have chosen your accessory and set up your communications, you may perform a final test to ensure that your system is performing properly. Click on **the Demo Mode** button so that it displays **Demo Mode Off.** Now click on **Initialize Motors**. The two indicators to the right of the Initialize button should turn green as the motors on your accessory are initializing. When the motors have completed their motions, the two indicators will turn blue. If you still have communications problems, these indicators will turn black and an error message will appear. You will then have to try other settings for your communications.

Demo Mode

You may have been sent this software for demo purposes. In order for the software to function correctly, you should click on the Demo button to change it to display **Demo On**. When this is done, the full functionality of the software is present, except that the software will not attempt to establish communications with the AutoPRO motion controller.

Startup Options

The way in which AutoPRO is run, and the information displayed, may be decided on by changing how AutoPRO is launched. The following configurations are available:

- **Normal**
  This is the usual way of running AutoPRO. If you do not specify any parameters then AutoPRO will start in this mode. The full capabilities of AutoPRO are available so that you can Define Custom Profiles, and set up your accessory, spectrometer and experiment.

- **Brief**
  This mode of operation is a simpler display. In this mode, you will be able to program profiles, choose a selection of profiles to use and run an experiment that has previously been set up. In this mode you will not be able to setup the accessory, spectrometer or experiment.

- **Simple**
  This is the simplest display. The only item that is displayed is a thumbnail of the profile selected. This mode is useful when AutoPRO is being controlled from an external program.

- **Minimized**
  The software may be run minimized. Again, this mode of operation is useful when an external program controls AutoPRO.

In order to customize your startup, follow the steps below:

1. Use My Computer to find the AutoPRO Program and create a shortcut. Click on the My Computer Item on the desktop. Select the drive in which you installed AutoPRO and then the folder that

contains the AutoPRO software. Click and hold down the mouse on the program named **AP5.EXE**. Drag the program to the desktop and let go of the mouse. You will now have a shortcut.

2. Using the RIGHT mouse button, click on the AutoPRO Shortcut on your desktop. When you click on AutoPRO with your right mouse button, a menu appears.

3. Click on the properties item at the bottom of the menu. A properties dialog box will be displayed. Two tabs are displayed at the top of the dialog box. One tab is called General, and one is called Shortcut.

4. Click on the Shortcut Tab. A text entry box named Target will be displayed. The target has to be modified by adding extra information called Command Line Arguments. For instance, your target text box may display: **C:\AutoPRO\ap5.exe**

5. Click to place the text insertion point at the end of the text string.

6. Type in the appropriate command line argument:

   - **To start AutoPRO in Normal Mode**
     You do not need to do anything. This is the default operation of AutoPRO. The target text Box should display

     C:\AutoPRO\ap5.exe

   - **To Start AutoPRO in Brief Mode**
     Change the target text box by adding a space followed by B

     C:\AutoPRO\ap5.exe B

   - **To Start AutoPRO in Simple Mode**
     Change the target text box by adding a space followed by S

     C:\AutoPRO\ap5.exe S

   - **To Start AutoPRO in Minimized Mode**
     Change the target text box by adding a space followed by M

     C:\AutoPRO\ap5.exe M

   The character added as a command line argument may be upper or lower case. There must only be one character used as a command line argument.

7. Click OK.

Security

AutoPRO has built-in security so that even if you wish to always run the software in normal mode, many of the functions of the software can be locked so that a password is required to change values. Only one password is used but you may decide which items you wish to have password protected.

On-Line

AutoPRO contains on-line help. You may enter the Help system in several ways. If you click on the Help button, a menu of Help options is displayed.

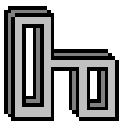
Customer Support

If you are in the U.S.A., contact PIKE Customer Support for assistance by the following means:

Phone: 1 (608) 274-2721
Fax: 1 (608) 274-0103
E-mail info@piketech.com
Web www.piketech.com

If you are outside the U.S.A., you may contact your local Distributor. A listing of all PIKE Distributors offices is available on our web site: www.piketech.com

AutoPRO Control



Introduction

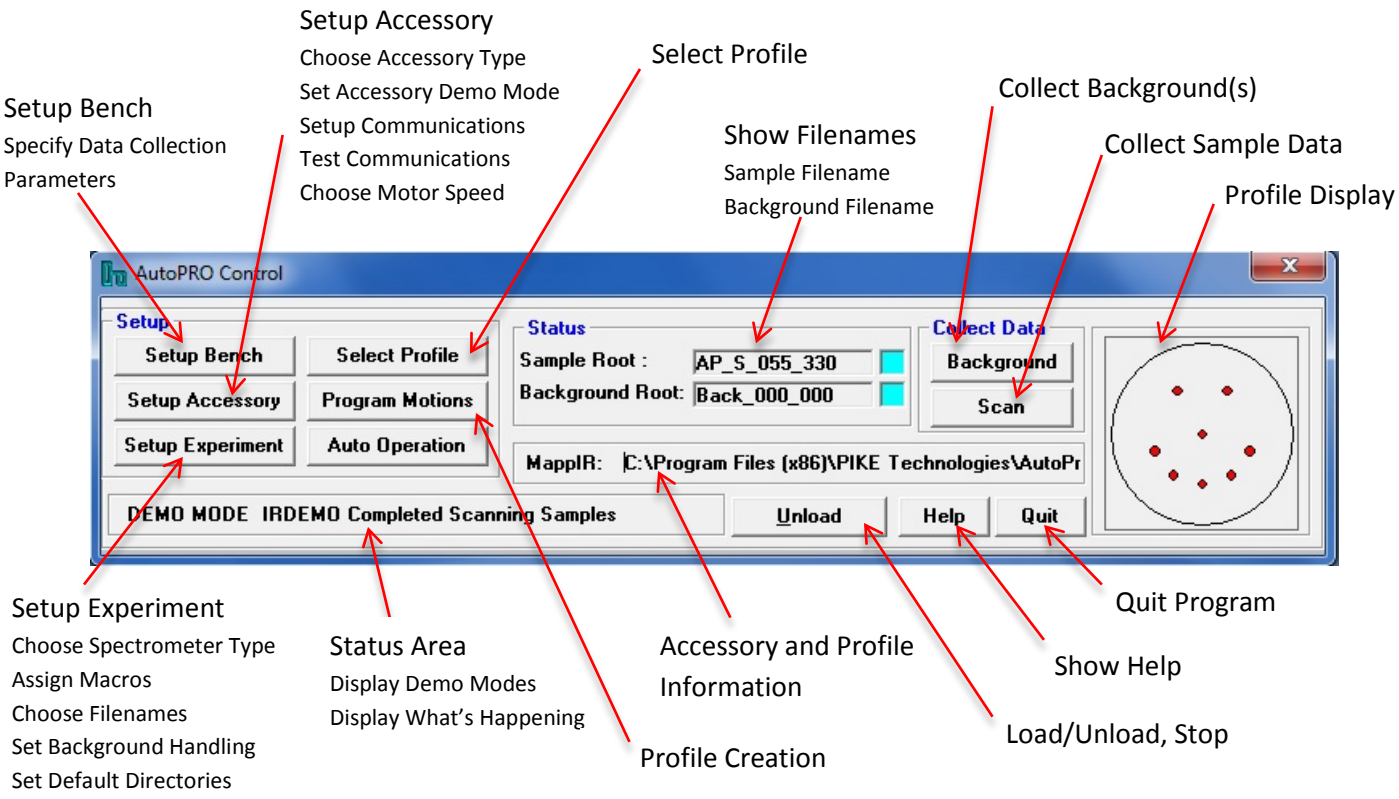
This chapter describes the features and operation of AutoPRO Control, the main Control Panel for your AutoPRO software. AutoPRO is unique in that it is an accessory automation software package, which may be configured for all the types of PIKE Technologies automated products. AutoPRO may also be configured to control most IR Spectroscopy packages to collect IR spectral information. Major features of this software package are:

- **Accessory interface**
  AutoPRO may be configured to operate all the varieties of automated accessories provided by PIKE Technologies. An accessory may be selected from a list of products. When this is done, the software configures itself to the particular automated accessory. This includes:
    - The mode of operation of the accessory.
    - Programming of the profile, a series of points or positions at which to analyze.
    - Display of the current profile selected.
- **IR Software Interface**
  The spectrometer and software package to be used is selected by clicking on a list of available IR software packages. Most software packages available today are supported. Basic data collection parameters such as resolution, number of scans, spectra format and spectral range may be set up to configure your data collection to your specific needs.
- **Dedicated Applications**
  The software may be configured to run a complete application. It is possible within the software to set up macros to be run to perform data setup, analysis and workup of results automatically.
- **External Control**
  It is possible to operate the software remotely through a dynamic data exchange interface so that an automated experiment may be run from within your IR software package macro capability.

Display Features

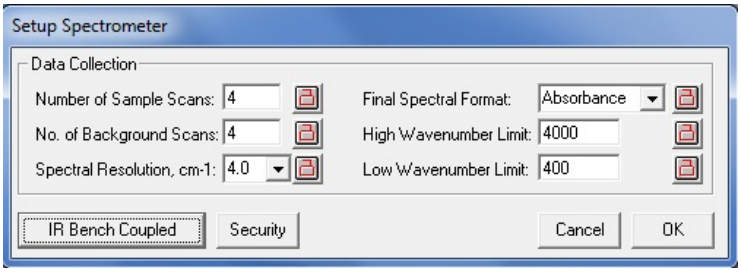
Major features of AutoPRO Control are described here. The normal display mode is shown.

When you start AutoPRO, the following display is shown at the bottom lower portion of your screen. Note that AutoPRO control does not use a standard pull down menu system. All the functionality of the software may be accessed by clicking on the buttons in the display.



Spectrometer Setup

This button opens a dialog to enable you to set up some of the data collection parameters for collecting data on your spectrometer.



There is a security feature on this page. Any of the six parameters may be locked, so they cannot be changed unless a password is supplied. In the display below, three items are locked and three items are unlocked. To change the security of a parameter, you must select security and enter a password. You will then be able to toggle the security status of a parameter by clicking on the padlock adjacent to it. Note that every time this display is opened, you must enter a password to change security settings.

The only parameters that are modified when you collect spectra with AutoPRO are the parameters shown. If you wish to set other parameters you may do either of the following:

1. Start your FTIR software package and set the parameters required before running AutoPRO. When AutoPRO collects data, it will only start your FTIR software package if it is not already running.

2. If you wish to fully automate the procedure of setting parameters:

    a. Run your FTIR Software package.

    b. Set the configurations that you wish to use.

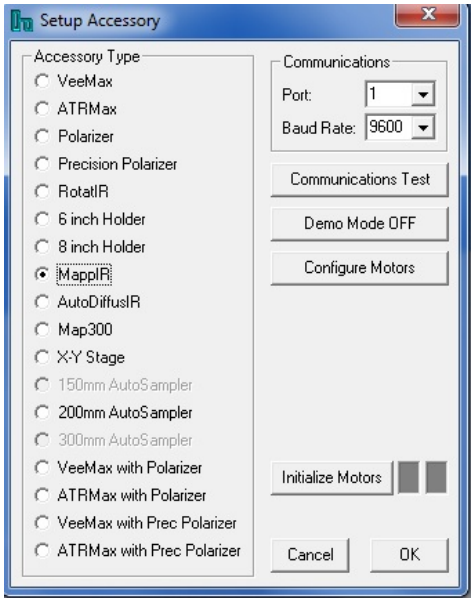
    c. Save this information in a parameter, experiment or settings file in your software. Each variety of FTIR Software has a different name for this file.

    d. Set up your software so that these settings are reloaded at startup.

On this page you are also able to decide whether you have a spectrometer attached. By clicking on the Bench Coupled button, you can select whether the bench is coupled or not coupled. This allows you to run the software on your office PC.

Accessory Setup

Clicking on the Setup Accessory button displays the dialog shown below. This display allows you to setup and configure all aspects of the operation of your accessory:



In order to select your accessory, click on the button next to the description of your accessory. All parameters and settings will be changed to reflect this choice.

Configure Communications

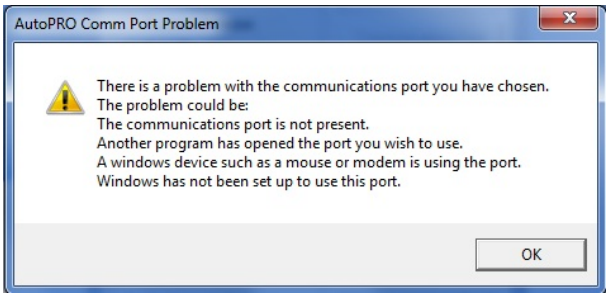
There are two settings that are required to configure communications; the Baud Rate and the Communications Port you wish to use.

Baud Rate

In most cases, 9600 baud may be used. If you experience communications problems, or are using a slower computer, you may need to select a slower baud rate. The AutoPRO controller will automatically adjust to the baud rate selected. You may select a baud rate between 2400 and 9600.

Communications Port

There is a choice of four ports that may be selected. Most PC's are equipped with two ports, Com1 and Com2. If you select a port that is not available on your computer such as Com1 when Com1 is not actually present, the following error box will appear.



Communications Test

Some of the computers that are sold today have two serial port connectors on the rear of the computer. However, in some cases, one of these connectors may not be internally connected. For instance, if an internal modem is fitted, this modem may be dedicated to Com2. If you have a problem establishing communications, a loopback connector is supplied with your accessory. This connector connects the transmit line to the receive line of the communications connector on your PC. To use this connector:

1. Plug the connector into the Com port that you wish to use.

2. Select the Com port in the software from the list provided.

3. Click on the **Communications Test** Button and the following box appears.

4. Click on the **Check Port** button. The software will first test to see if the port is present. If the port is not present, the error message shown below will appear. If the port is present, the software configures the port and sends a message out on the transmit line of the port. Since the loopback connector connects the transmit and receive lines of the communications port, this test message should appear on the receive line. If the software does not receive this message, the following error is displayed.

If you see this message, the communications port that you wish to use is not internally connected. You must review the User manual that came with your computer, or try another port. If the test is successful, the following message will appear.

You have now successfully established a communications link between your computer and the AutoPRO motion controller. The next time the software is run it will default to this new configuration.

NOTE: Remember to remove the loopback connector after completing this test!

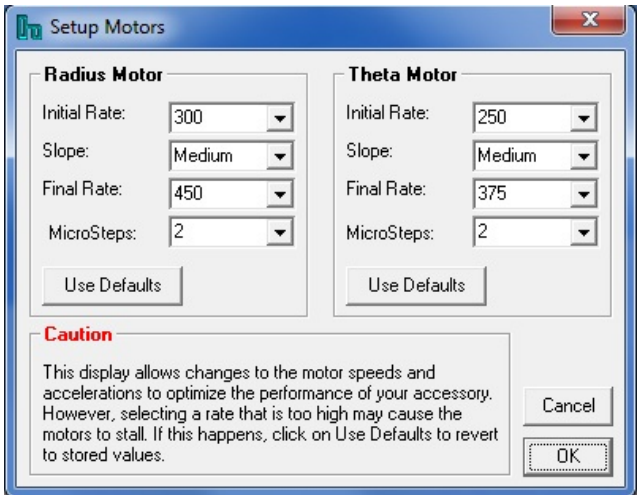
Now that you have chosen your accessory and set up your communications, you may perform a final test to ensure that your system is performing properly. Click on **the Demo Mode** button so that it displays **Demo Mode Off.** Now click on **Initialize Motors**. The two indicators to the right of the Initialize button should turn green as the motors on your accessory are initializing. When the motors have completed their motions, the two indicators will turn blue. If you still have communications problems, these indicators will turn black and an error message will appear. You will then have to try other settings for your communications.

Demo Mode

You may have been sent this software for demo purposes. In order for the software to function correctly, you should click on the Demo button to change it to display **Demo On**. When this is done, the full functionality of the software is present, except that the software will not attempt to establish communications with the AutoPRO motion controller.

Configure Motors

The default speeds that are set when you run your accessory are conservative values. You may click on the Configure Motors button to speed up your motors. Care must be taken when doing this since too fast a speed may stall the motors. If this is the case, click on the Use Defaults button to restore the default speeds.



Initialize Motors

This button allows you to initialize your accessory. This function is useful when setting up your communications settings. There are two indicators to the right of this button which are motor status indicators.

The number of motors used will depend on the type of accessory selected. If a motor is not present in the accessory, the corresponding block will be disabled and will appear gray. The blocks display a color code depending on the status of the motors. These colors are:

Black

The communications with the motor controller have failed. This color will be present if the motor controller is not connected, not switched on, or if the communications parameters have been changed without cycling the power on the controller box.

Green

The motor has been initialized correctly and is moving.

Cyan

The motor is initialized correctly and has stopped moving.

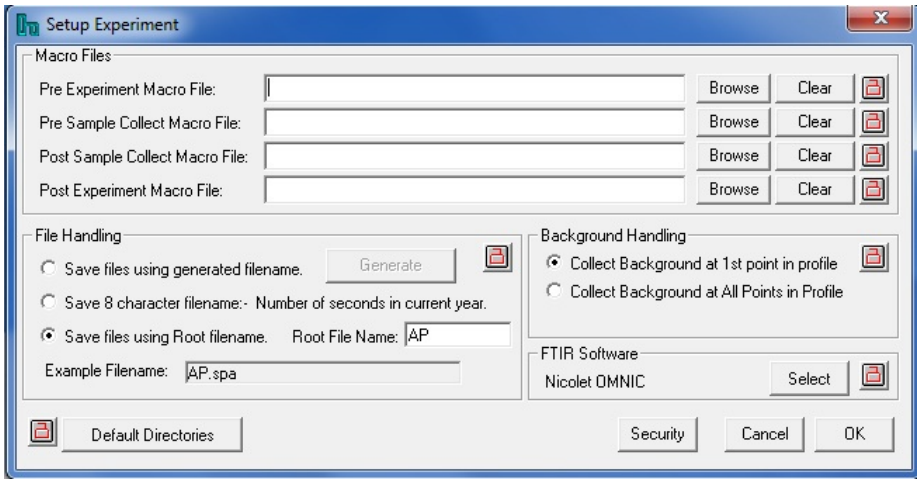
Grey

No motor present.

Experimental Setup

This display allows you to set up a complete experiment. On this page you can:

- Select an FTIR Spectrometer to use.
- Select default directories to save and retrieve:
  - Profiles
  - Spectra
  - Macros
- Decide on how to automatically name your spectral files.
- Decide whether you wish to collect multiple backgrounds.
- Set up four Macro files.
- Choose which of the above items are locked/unlocked with security.



Macro Files

You can set up an experiment or design a customized application. In the display above, the Macro File items have been locked so that they cannot be changed without knowing a password. These items have been assigned to a specific macro file. The Pre-Experiment Macro File sets up the configuration for the experiment, including loading a quant method, and opening an Excel spreadsheet file to receive the quant results. The second Pre-Sample Collect Macro File is used to set specific parameters prior to collecting each sample spectrum. The Post-Sample Collect Macro File is used to perform a quant on the data collected and place this data into the Excel Spreadsheet. The Final Post-Experiment Macro File is for program cleanup, such as saving the Excel file with its results.

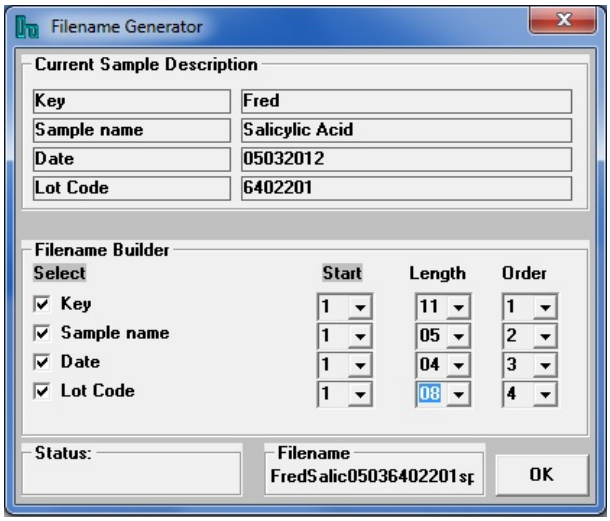
File Handling

The file handling area is used to enable you to automatically name spectral files so that you can save the data with unique names.

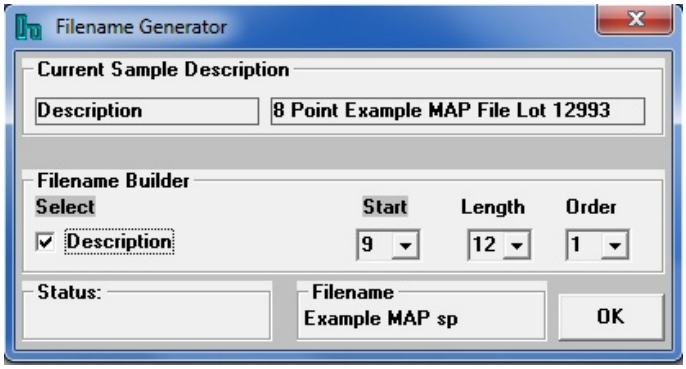
There are three ways in which you can name your files. In all cases an example of the filename that you will be using as a base or root filename is shown. When you collect data, the background file is named “back”. If multiple backgrounds are collected, they are appended with a three digit numerical extension. The sample file is named by appending a three digit numerical extension to the root.

If you use the Base filename option, enter a base filename into the text box. When this feature is selected the saved spectral file name will be the base plus a “B” indicating background or “S” indicating sample plus the Radial distance plus the angle. For example, test S 046 270 indicates the sample spectrum was collected at radius = 46 mm at an angle of 270°. You may also generate an eight character numeric filename which is just the number of seconds in the current year. This method of naming will ensure that each sample that you collect will have a unique name.

Finally you may generate a filename automatically, based on the information that you entered into your Profile. For the Auto DiffusIR and XY Stage you may use the information that is contained in the sample information fields. For the other programmers, part of the description field may be used.



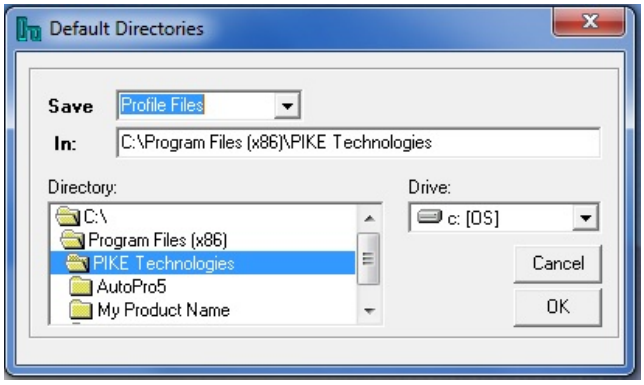
In the case shown, the information entered into an Auto DiffusIR file is shown and consists of four fields. To generate a filename, we have selected the 11 characters of the key or operator name, 6 letters from the sample name, 4 from the date field and 8 from the lot code field to form our unique filename. Any characters in any field may be used in any order to form this filename. If we are using one of the other accessories, such as a MappIR, only the description field is used. In this case, each individual file will be appended with a three digit numeric equal to the position of the sample in the MappIR Profile.



In this example the lot number has been selected as a root filename.

Default Directories

The directories that you wish to save information in may be defined by using the default directory button. The default location of three types of files may be decided on. These are Profiles, Spectra and Macros.



Note that when you use a programmer for defining the points to analyze, the default profile directory that you define here is used when saving the profile as the initial directory in your file save dialog.

Background Handling

For some automated accessories, you are able to decide whether you wish to collect a background at the first point in your profile or at all points in your profile. You are not allowed to make this choice for the following accessories:

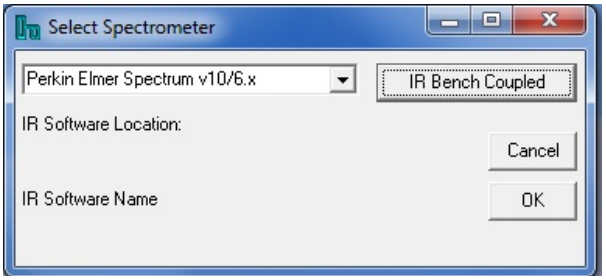
- **Automated Disk Checker**
  You have to collect background spectra at every point in your profile. This is because the automated disk checker experiment is a very sensitive measurement. The analysis is performed at an 80° angle. Since, for most types of hard disk, the background spectrum changes slightly with respect to radial position, collecting background spectra at all points results in more accurate results.

- **Auto DiffusIR**
  When using this accessory the background sample is defined as the sample at the center of the sampling plate. Thus there is only one background sample. In this case, you are not allowed to collect backgrounds at all sample positions.

- **VeeMAX, ATRMax, and Polarizer**
  For the VeeMAX accessory the background sample is usually a gold mirror. For the ATRMax accessory the background spectrum is of a clean ATR crystal. For the Polarizer accessory the background sample is nothing for a transmission experiment. In these three cases, spectra are collected at different angles. Since the background spectrum varies depending on the angle that is set, a background spectrum must be collected for all sample positions in the profile.

FTIR Software

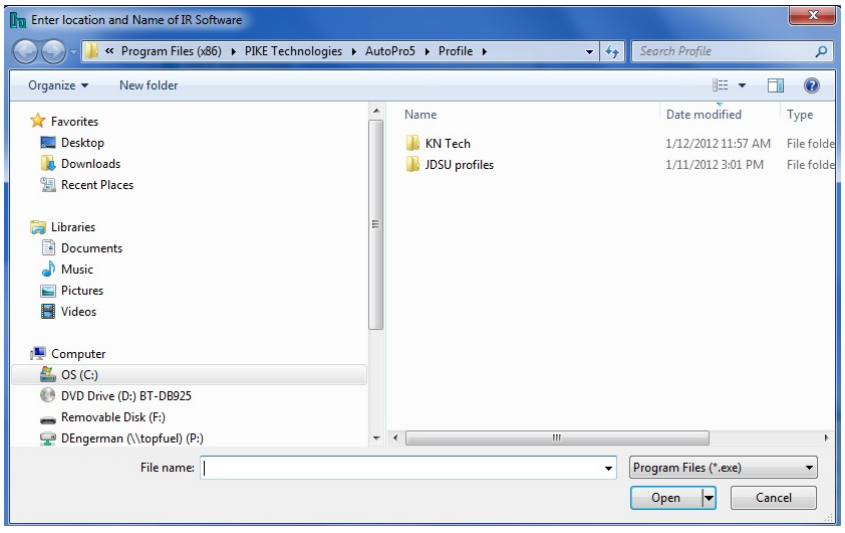
AutoPRO control includes software to interface your automated accessory to most Windows based FTIR software packages. In order to pick a software package, click on the **Select** Button. The dialog below will open.



When you click on the down arrow a list of FTIR software packages will be displayed. This list includes (in alphabetical order):

Agilent Resolution PRO	Bomem GRAMS	Mattson WinFirst
Bio-Rad Merlin	Bruker OPUS	PerkinElmer Spectrum v5, 6 and 10
Bio-Rad Win-IR	Midac GRAMS	Shimadzu Hyper-IR
Bio-Rad Win-IR PRO	Nicolet OMNIC	

Select one of these software packages. You will then be asked to find the directory and executable program which runs when you launch your software.

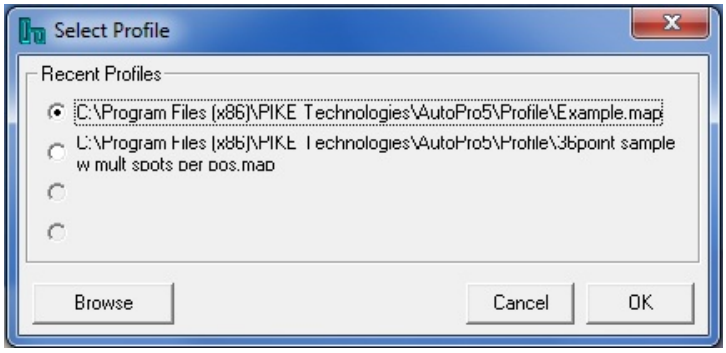


This step has to be performed since your software could be installed in a user named directory.

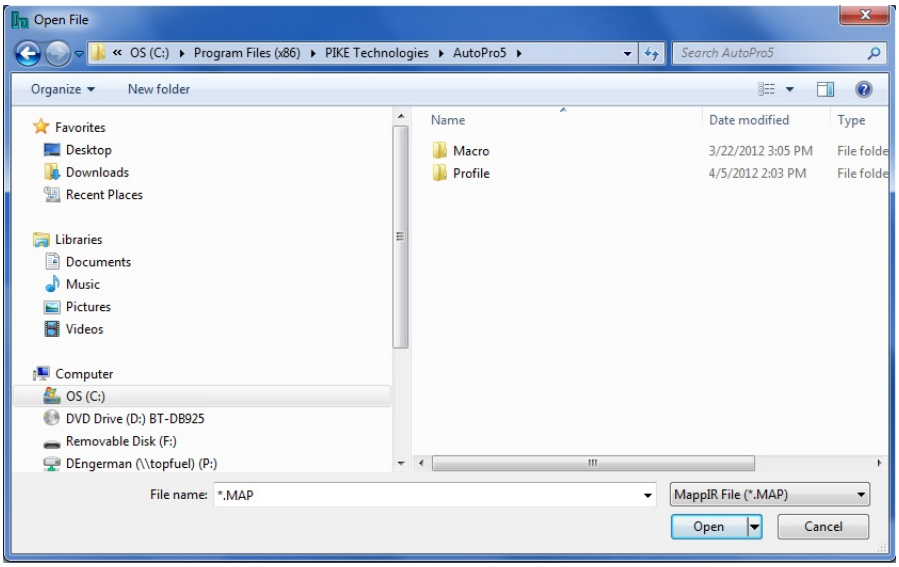
Several of the software packages do not allow the location of the software to be determined automatically. Once you have made your selection, the software remembers your choice.

Select Profile

When you click on the Select Profile button, a choice box will open. The last four profiles that you have used will be displayed.



You may pick one of these profiles, or click on the Browse button to load a different profile.



When a new profile is loaded, it is placed in the first position. The fourth profile name is deleted and the other profiles are moved down the list.

Program Motions

You may run the Profile Programmer for your accessory by clicking on this button. The programmer will open and you will be able to define a new profile. Clicking this button opens the AutoPRO programmer. This programmer changes depending on the accessory selected:

- For the VeeMAX, ATRMax, Polarizer and RotatIR, a common program, AutoPRO/Max is used.
- For the 6 inch wafer holder, 8 inch wafer holder, MappIR and MAP300 accessories, the programmer is AutoPRO/Wafer.
- For the Auto DiffusIR accessory, the programmer is called AutodiffusIR.
- For the XY Stage, the programmer is called AutoXY.

Details of how to use the Profile Programmers are given later in this manual.

Status Area

This area gives information on the following:

ACCDEMO	If displayed, the accessory is in demo mode.
IRDEMO	If displayed the IR bench is not coupled.
Data Collection Status	The progress of your data collection is displayed here. This includes whether you are collecting a background or a sample and the current point in the profile.
Accessory Status	The progress of your accessory is displayed here. This includes whether the accessory is initializing or moving to a point.

Filename Area

The filename that is used to save your data is shown here.

Accessory/Profile Area

The accessory type and filename of the current profile is displayed here.

Collect Data Area

Clicking on Sample or Background will initiate data collection. The sample Button is grayed-out until a background has been collected. When the background button is clicked, if your FTIR software is not running, it will be launched. Some software will launch in a maximized window. If this is the case, it is useful to click the restore button and reduce the size of the window so that both AutoPRO and your FTIR software package are both visible on the screen.

Motor Status

This area displays information on the communications between the computer and the Motion controller. The number of motors used will depend on the type of accessory selected. If a motor is not present in the accessory, the corresponding block will be disabled and will appear gray. The blocks display a color code depending on the status of the motors. These colors are:

Black

The communications with the motor controller have failed. This color will be present if the motor controller is not connected, not switched on, or if the communications parameters have been changed without cycling the power on the controller box.

Green

The motor has been initialized correctly and is moving.

Cyan

The motor is initialized correctly and has stopped moving.

Grey

No motor present.

Unload

For the wafer holder, Multisampling, MappIR and AutodiffusIR accessories, the accessory may be moved to an unload position to simplify the insertion of new samples.

This button unloads the accessory and is used for the 6 and 8 inch wafer holders, MappIR, Map300, AutodiffusIR, XY Stage and Disk Checker. When the unload button is clicked, the accessory is moved to the unload position, the Button legend is changed to Load and all other buttons except Quit are disabled. If the button shows load and is clicked, the accessory will move to home position and all buttons will be enabled.

The function of this button changes when data is being collected. This button is then used to stop a data collection process. The system will not stop immediately, but after any data collection has completed.

AutoPRO Wafer Programmer

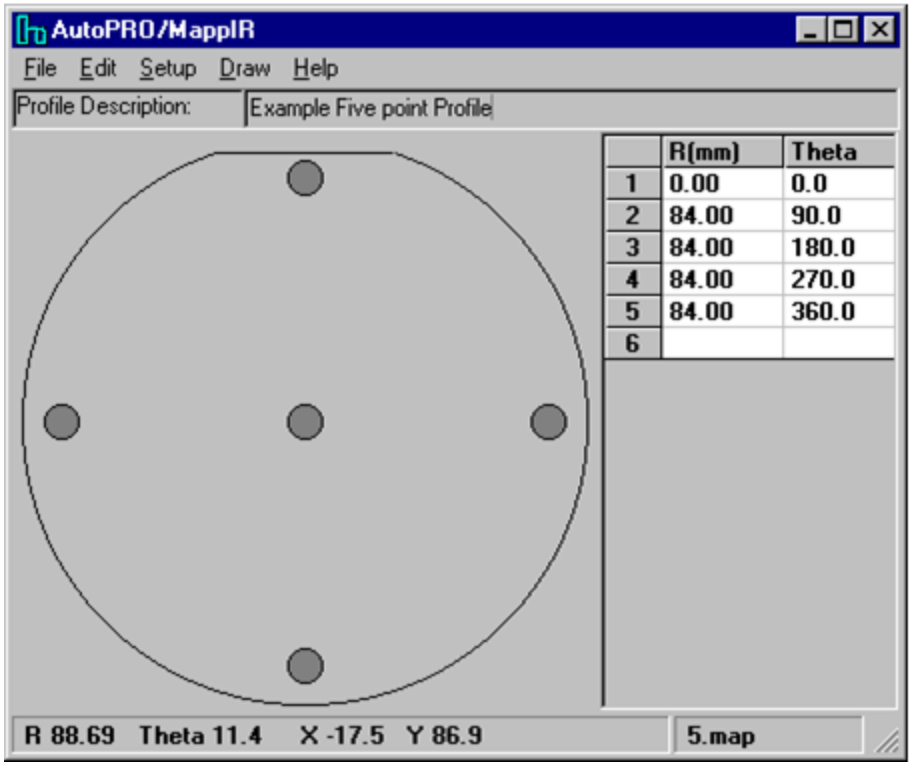
Introduction

AutoPRO Wafer is the programmer that is used for the following accessories:

- 6 inch wafer holder
- 8 inch wafer holder
- MappIR
- MAP300

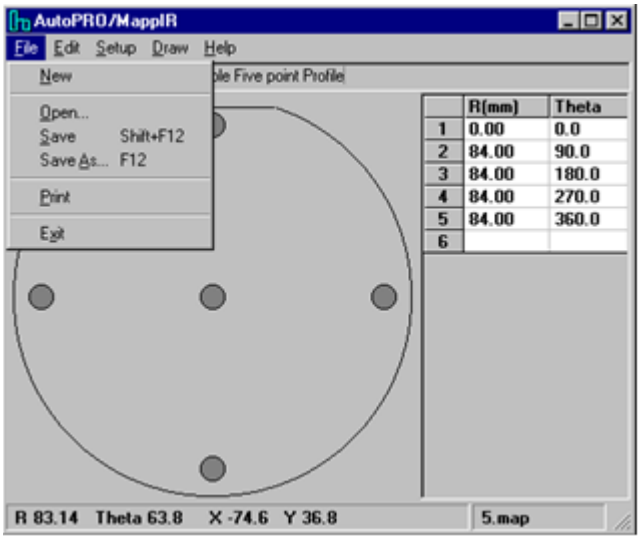
The AutoPRO Wafer programmer allows a series of positions to be analyzed on a sample. The positions of the points to be analyzed are defined in terms of R-Theta or Cartesian coordinates. Points may be placed in a random manner. Also several fixed patterns are available such as a five, nine or seventeen point pattern. Points may also be placed in a regular R-Theta or X-Y grid pattern. Up to 2000 points may be placed on the sample.

This chapter gives a general description of each menu and the commands available.



File Menu

This menu is used for saving and retrieving sampling configurations. The data shown on the screen may also be printed to your default Windows printer.

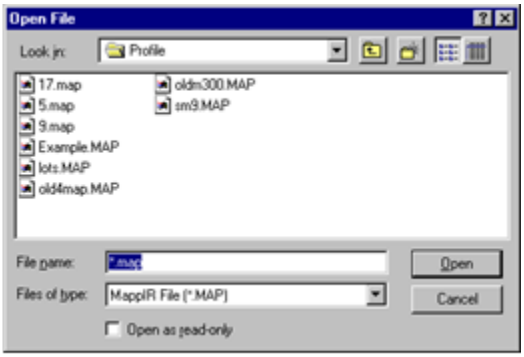


New

The **New** command clears the wafer, data and file areas. If there are any unsaved changes when you select the New command, AutoPRO asks if you want to save the changes.

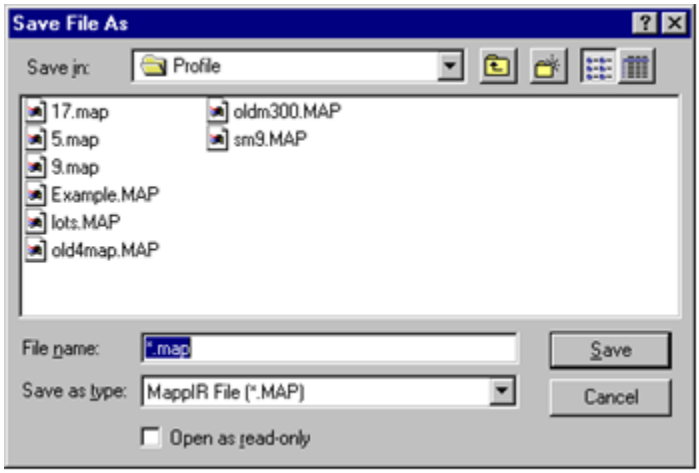
Open

The **Open** command loads a file that was previously stored on disk. The Open Dialog is displayed and you may choose the directory and file that you wish to load. The opening directory used in the Open File dialog is the one that is specified in AutoPRO control. If a default directory has not been specified, the opening directory location is the same directory as the one that holds the AutoPRO Wafer executable program. The file name extension used in this dialog box is dependent on the accessory that you are using. For the 6 and 8 inch wafer holders, the extension is *.WAF. For the MappIR accessory the extension is *.MAP.



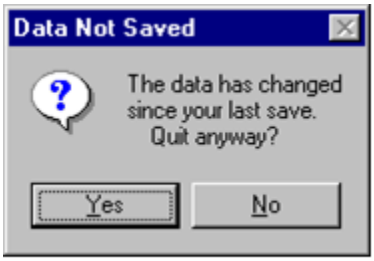
Save
The **Save** command saves your work in a file. If the File Status is clear, indicating that the file has not been named, the Save File Dialog box appears so you can give your file a name.

Save As
The **Save As** command saves your work. The **Save File As** dialog box appears so you can save your work with a different file name. The opening directory used in the Save File dialog is the one that is specified in AutoPRO control. If a default directory has not been specified, the opening directory location is the same directory as the one that holds the AutoPRO Wafer executable program. The file name extension used in this dialog box is dependent on the accessory that you are using. For the 6 and 8 inch wafer holders, the extension is *.WAF. For the MappIR accessory the extension is *.MAP.



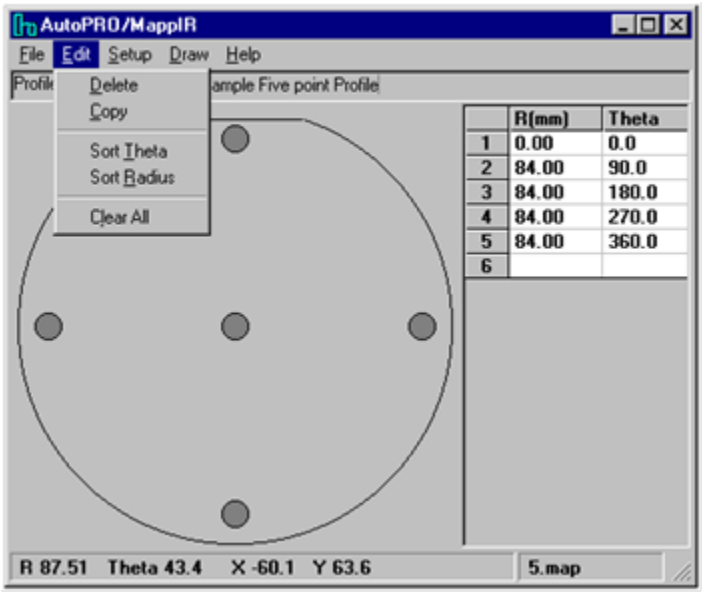
Print
The **Print Data** command prints the data.

Exit
The Exit Command closes AutoPRO. If the data has changed since your last save, AutoPRO prompts you to exit anyway or cancel the Exit Command.



Edit Menu

These menu items are a set of functions which are used to reorganize the data.



Delete

This command deletes the data that is highlighted in the data area.

Copy

This command copies the data to the clipboard for use in other applications. Using the mouse, highlight the data in the data area. Selecting **Copy** will place this data on the clipboard. The data may then be pasted into other applications by choosing the **Paste** function in the other software.

Sort Theta

This command allows you to reorder the points on the wafer. During analysis the wafer is moved sequentially from point to point starting at point 1. The **Sort Theta** item allows you to sort the points in terms of increasing theta.

Sort Radius

The **Sort Radius** item allows you to sort the points in terms of increasing radius.

Clear All

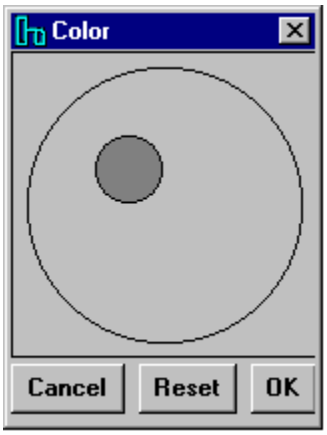
This command clears the wafer and data areas. If this data was displayed from a file, the filename will not be cleared.

Setup Menu

This menu has two items to set basic parameters to change the color of the display and set the edge exclusion and spot size.

Color

This command changes the color of the display. The wafer or spot may be individually changed to a different color. You may change colors, save new color patterns, or reset the display to its' original colors.



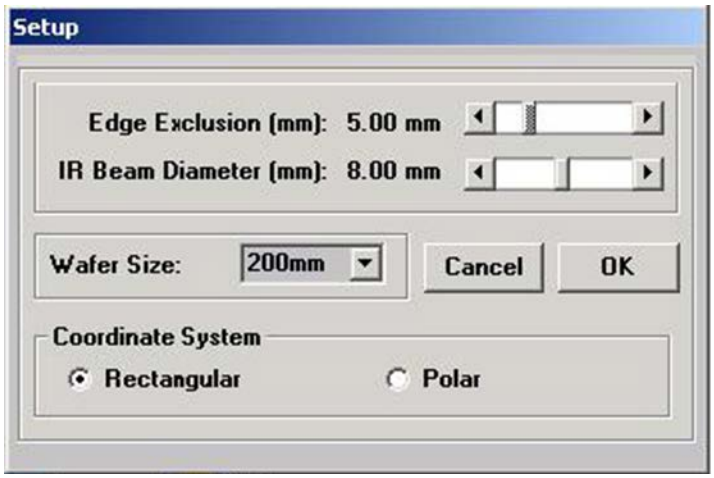
To change the default colors, double click on either the large or small circles. The large circle represents the wafer, or background, while the small spot represents the analysis spot. The **Color Box** will appear, allowing you to select a different color.

Reset

If you wish to return to the colors originally provided by AutoPRO select **the Reset Colors** button. The wafer will become light gray and the analysis spot will become dark gray.

Parameters

Basic wafer parameters may be changed by selecting this menu. Note that if some spots are currently drawn on the wafer, the edge exclusion and wafer size cannot be changed. To change these parameters, the analysis pattern must be cleared by selecting Clear from the Edit menu or New from the File menu.



Edge Exclusion

Points will not be drawn in the edge exclusion area and the motors will be unable to move to this area.

IR Beam Diameter

This changes the spot size on the screen to show you how large the IR beam is on the wafer. Set the spot size to correspond to the diameter of the beam focus in your FTIR instrument.

Wafer Size

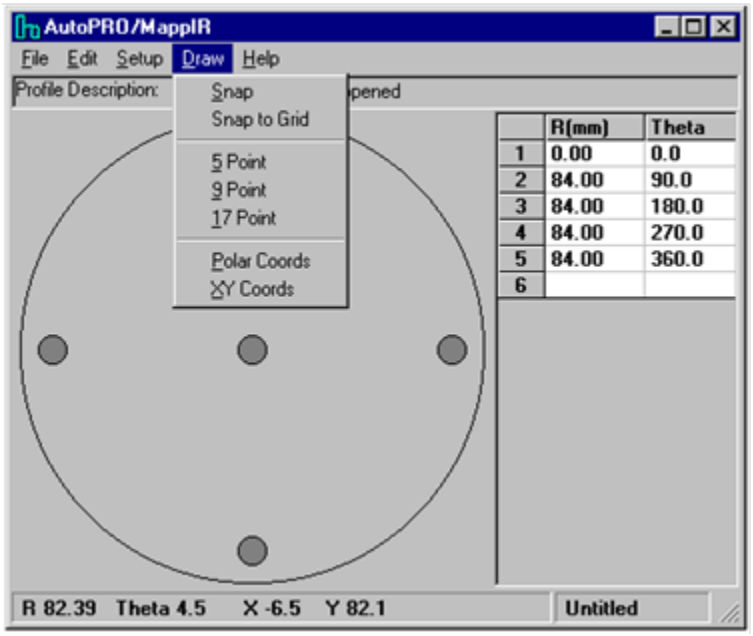
Several different diameters may be chosen. The drawing on the screen will be scaled to this diameter depending on the size of the wafer being analyzed.

Coordinate System

Select which coordinate system to use. This can be changed at any time and the data grid will be updated. Rectangular is the same as Cartesian. Polar coordinates are defined as a length and an angle (vector).

Draw Menu

The draw menu allows the operator to select either a grid or several pre-defined patterns. The exclusion parameter and spot size must be defined in the parameter menu and these will be used when calculating the positions at which the points are drawn.



Snap

This menu item allows points to be snapped to the grid defined in the **Snap to Grid** menu.

Snap to Grid

When this menu item is checked, a snap grid pattern may be defined. Using the slide bars for angle and radius, select the grid that you require. Select OK and a grid point pattern will be place on the wafer. Placing points manually will automatically move the point to line up with this grid.

5 Point

Clicking on this menu item draws a five point pattern on the wafer.

9 Point

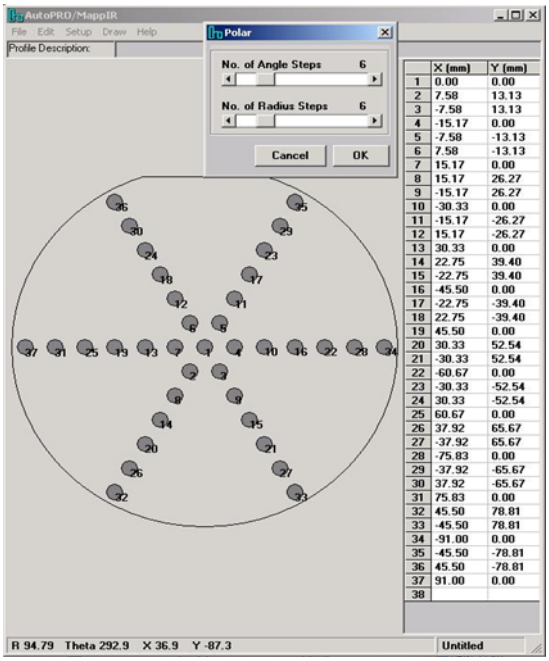
Clicking on this menu item draws a nine point pattern on the wafer.

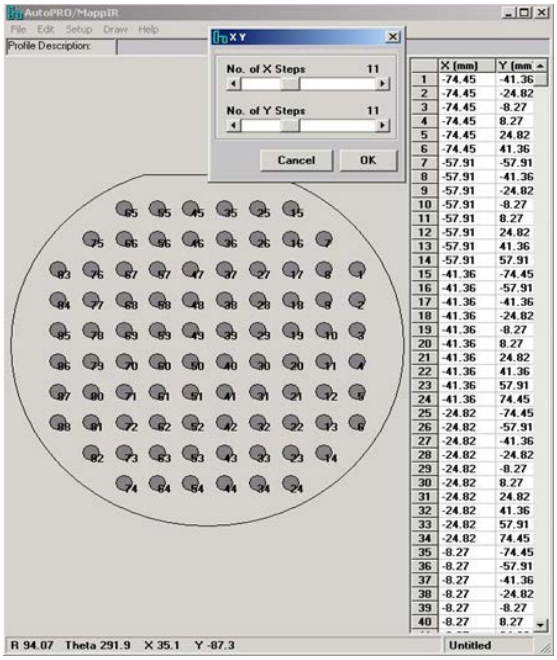
17 Point

Clicking on this menu item draws a seventeen point pattern on the wafer.

Polar or XY Coords

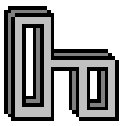
This will setup a “best fit” of an equal-spaced grid of points defined.





Manually Placing Points

Points may also be placed on the wafer manually in any order. Move the crosshairs to the desired position and click. Points may be removed by clicking on the point to be removed. Holding down the mouse button, the cursor is dragged outside the wafer area and the mouse button is then released. The selected point is removed from the wafer. The data in the data area is deleted.



AutoPRO Max Programmer

Introduction

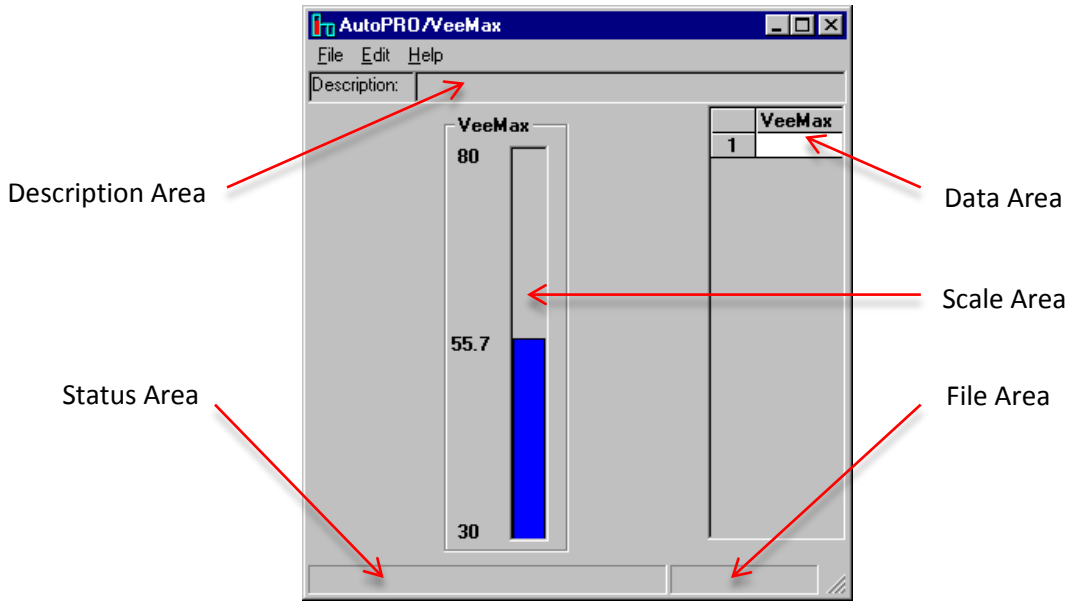
If you are operating an automated VeeMAX, ATRMax, Polarizer or RotatIR, the AutoPRO/Max Programmer will be displayed when you click on the program button. The operation of this program is identical for these three accessories, except for the high and low angle limits. For these three accessories, these limits are:

- VeeMAX 30° to 80°
- ATRMax 20° to 70°
- Polarizer/Precision Polarizer 0° to 360°
- RotatIR 0° to 360°

Note that if you are using a VeeMAX accessory and set up AutoPRO control for an ATRMax accessory, although the programmer will look similar, the conversion routines to convert from angle to number of steps are different for the different accessories.

The operation of the VeeMAX accessory will be described here for clarity. The operation of the other accessories is identical.

Sections of the Display



Status Area
This area of the screen displays status information on the position of the cursor. When the cursor is in the Scale area, the coordinates of the cursor on the wafer are displayed. These numbers displayed are updated only when the cursor is in a blue portion of the scale.

Scale Area
This area of the screen displays a graphical representation of the angle of the accessory. Analysis angles may be added to the list in the angle area by clicking on the mouse in the **Scale Area.**

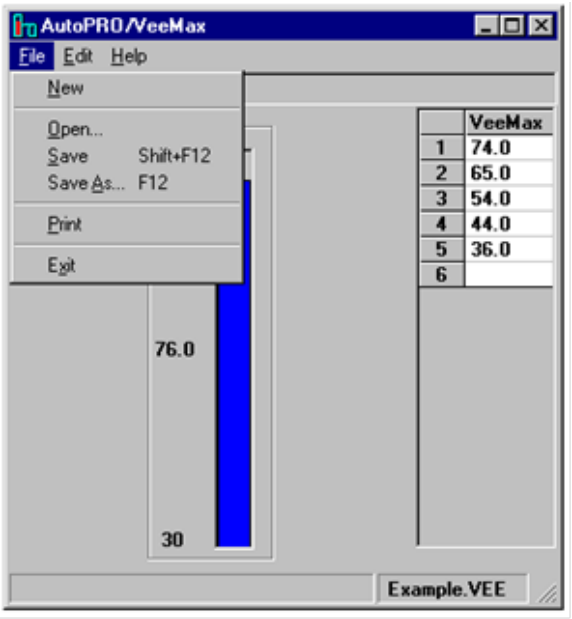
File Area
This area displays the current filename, selected by using the **File Save** or **File Open** command.

Data Area
This area of the screen displays the angle to which the accessory will be moved to. The data list may be scrolled to see all the data. Points may be added to the Data Area by typing coordinates into an empty cell. Points may be deleted from the data area by clicking on the cell at which the change is to be made, and then selecting **Delete** from the **Edit** Menu.

Description Area
You may enter a description on the sample that you are running in this text box. This description is used as the basis for automatic file generation in the AutoPRO Control program, so it is useful to enter a meaningful description here.

File Menu

This menu is used for saving and retrieving sampling configurations. The data shown on the screen may also be printed to your default Windows printer.



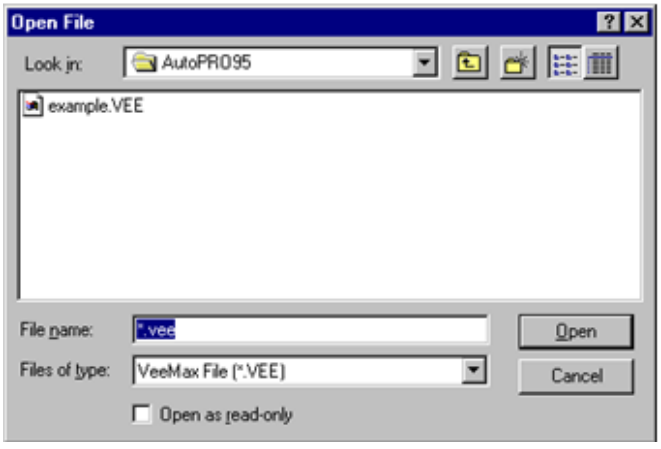
New

The **New** command clears the angle data. If there are any unsaved changes when you select the New command, AutoPRO asks if you want to save the changes. The filename is set to “Untitled”.

Open

The **Open** command loads a file that was previously stored on disk. The Open Dialog is displayed and you may choose the directory and file that you wish to load. All valid files have an extension which relates to the accessory you are using.

- For VeeMAX, the extension is *.VEE
- For ATRMax, the extension is *.ATR
- For the Polarizer, the extension is *.POL
- For the RotatIR, the extension is *.ROT

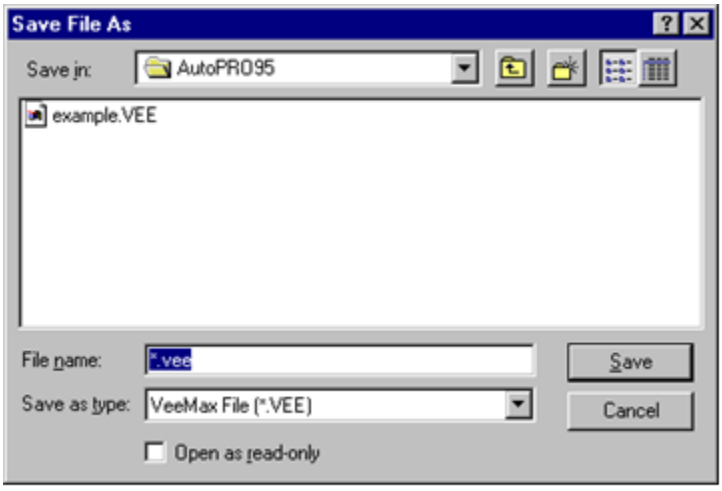


Save

The **Save** command saves your work in a file. If the File Status is clear, indicating that the file has not been named, the Save File Dialog box appears so you can give your file a name.

Save As

The **Save As** command saves your work. The **Save File As** dialog box appears so you can save your work with a different file name.



Print

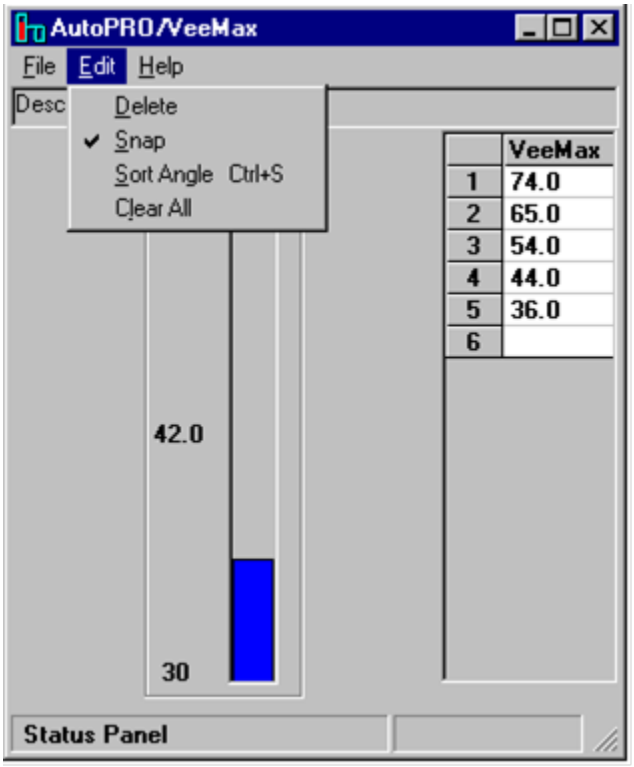
The **Print** command prints a list of the data that you have entered.

Exit

The Exit Command closes AutoPRO. If the data has changed since your last save, AutoPRO prompts you to exit anyway or cancel the Exit Command.

Edit Menu

These menu items are a set of functions which are used to reorganize the data.



Delete

This command deletes a line in the angle display at the current entry point. All remaining points in the angle table are moved up one place.

Snap

When snap is selected, the entries made in the angle table due to a mouse click on the display are rounded to the nearest degree.

Sort Angle

This command allows you to reorder the points in terms of increasing angle.

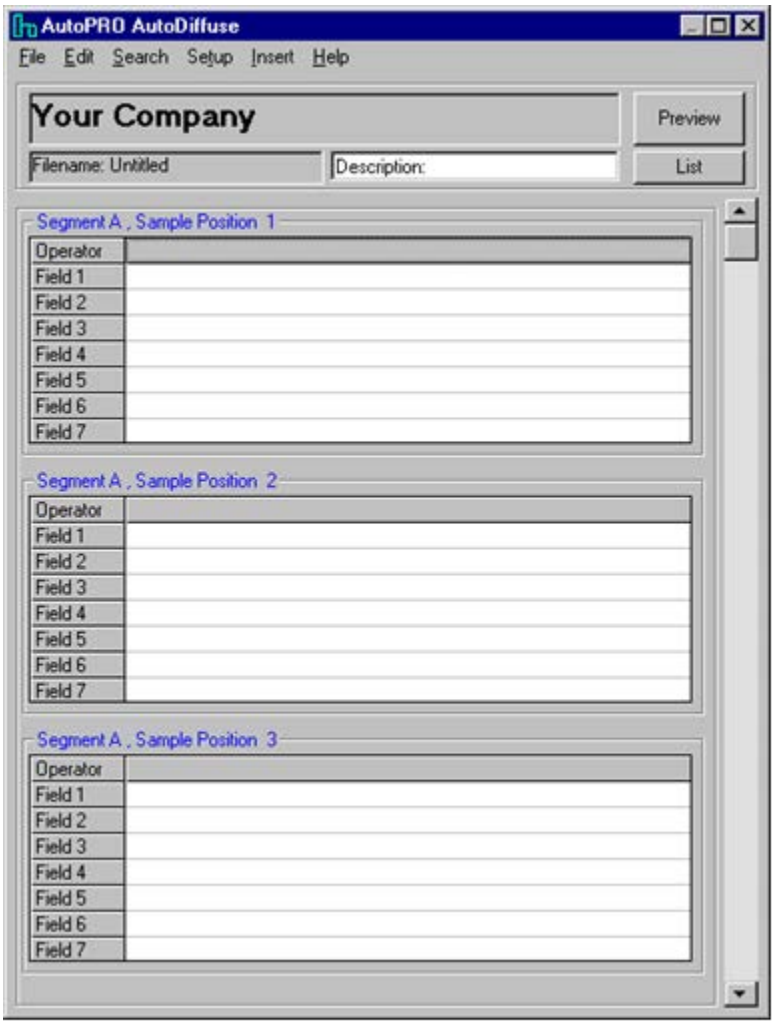
Clear All

This command clears the angle data. If this data was displayed from a file, the filename will not be cleared. When changes are made after clicking on this item, they may be saved to the same filename by selecting **Save** from the File menu.

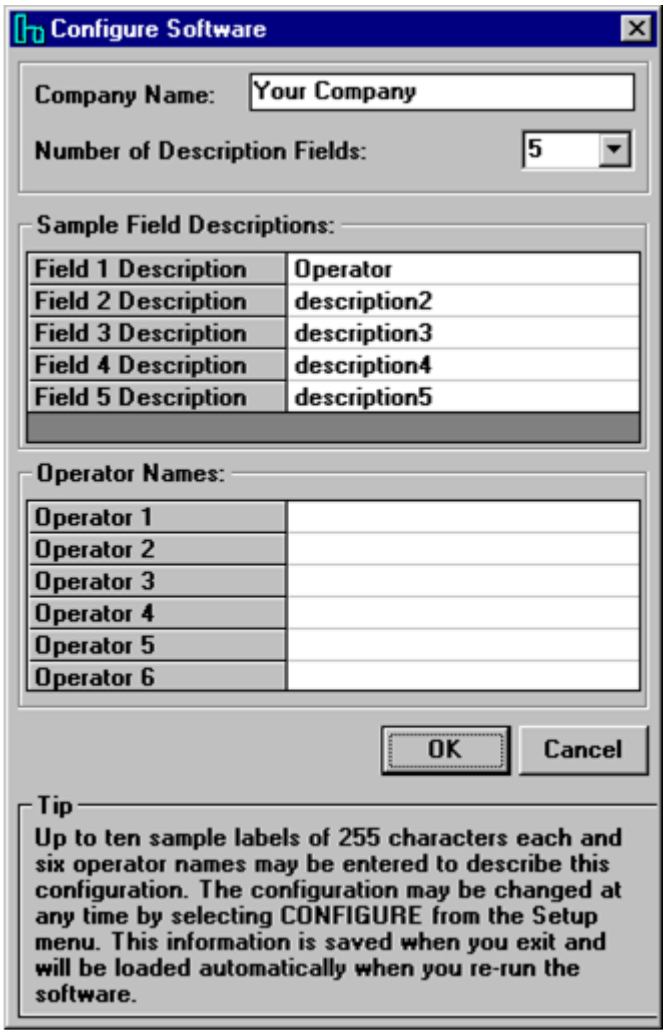
AutoDiffusIR Programmer

Introduction

The AutoDiffusIR programmer is used in conjunction with the PIKE AutoDiffusIR Accessory. This program allows the user to assign information to each sample being analyzed. Both an operator name and sampling information may be assigned to each sample in a point and click environment. The information, once entered, may be reviewed to ensure accuracy, printed out to provide a hard copy, and saved to disk in order to perform the experiment.



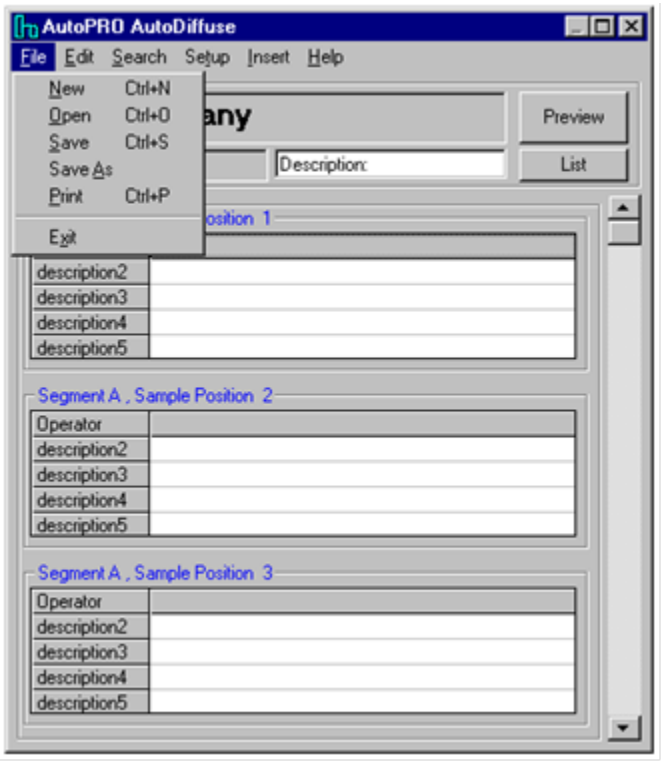
When the software is run for the first time, the configuration screen below is shown. The user may enter information to customize the software to his or her needs.



The company name may be set as well as the descriptions for the fields to be assigned to the sample. Up to six operator names may also be entered.

At any time this configuration screen may be accessed by selecting configure from the setup menu.

File Menu

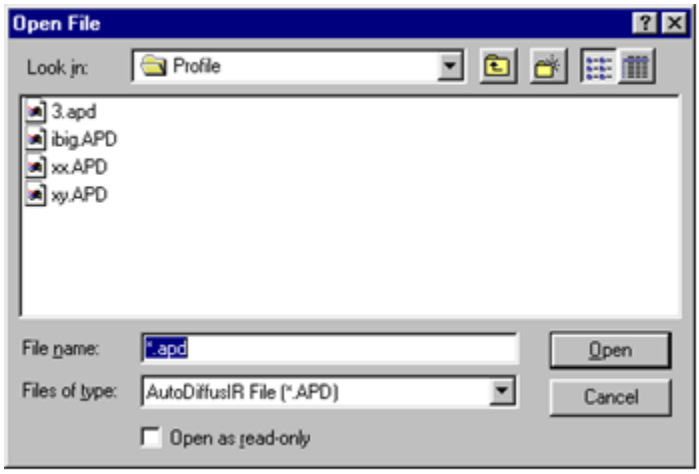


New

This command clears all data. If there are any unsaved changes when you select the New command, the software asks if you want to save the changes. The data is then cleared and the Title bar is changed to [Untitled.APD].

Open

This command loads a file that was previously stored on disk. The Open Dialog is displayed and you may choose the directory and file that you wish to load. Valid files have an *.APD extension.

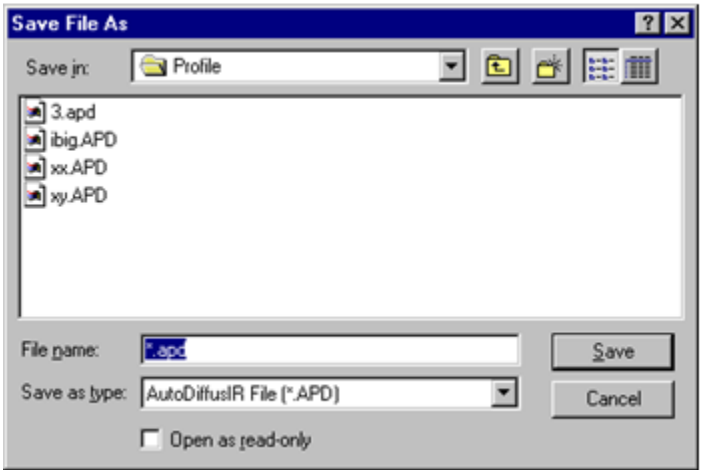


Save

This command is only enabled if a title is assigned to a file. If the file name is [Untitled.APD] this command is not available.

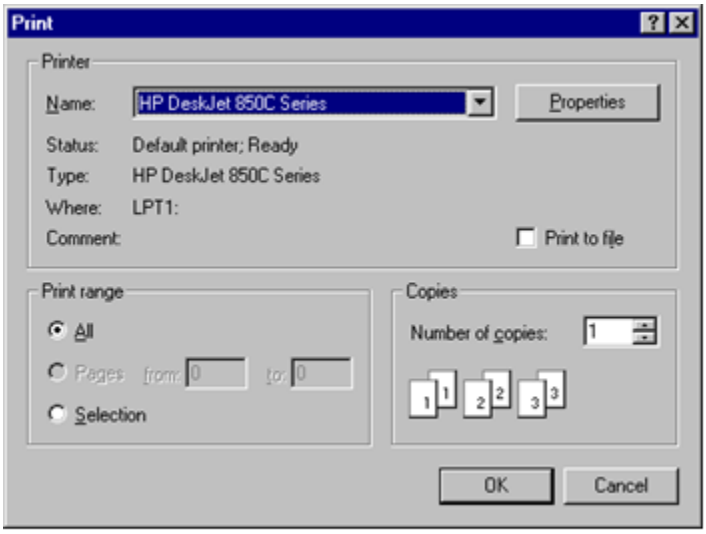
Save As

This command saves your work. The **Save File As** dialog box appears so you can save the file with a different file name, or save an untitled file with a new file name.



Print

This command prints the data in the data area. When selected the display below is shown.

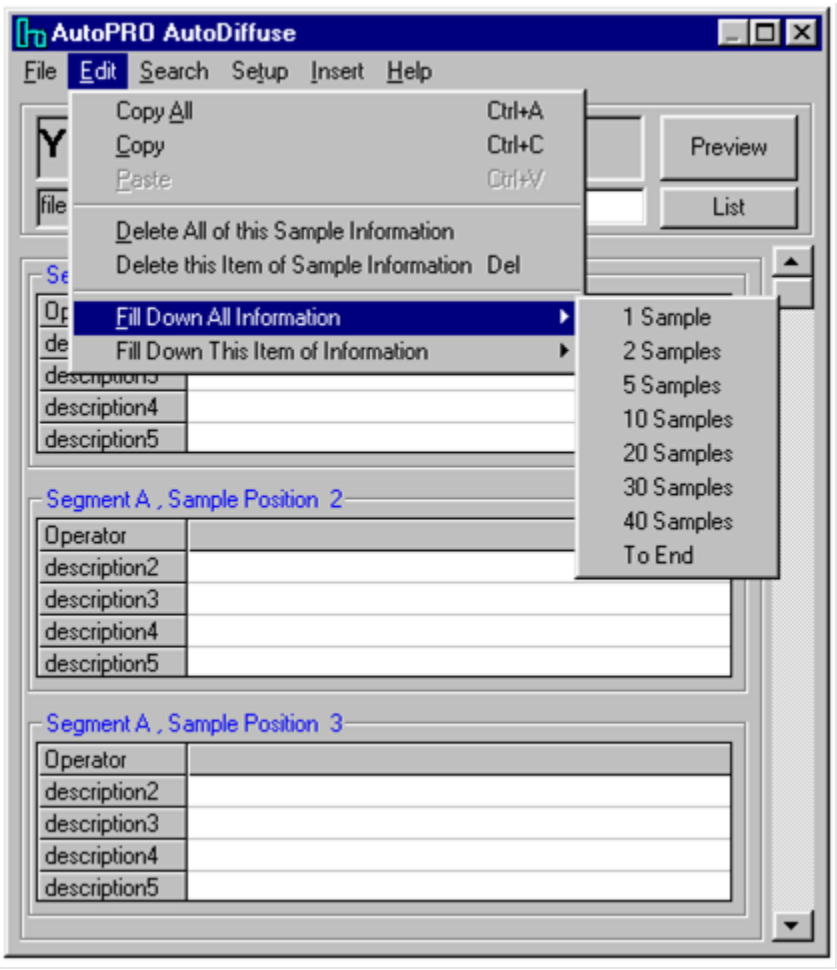


The font type and font size may be selected prior to printing. The page to be printed may be viewed by selecting Preview.

Exit

This command closes AutoPRO. If the data has changed since your last save, AutoPRO prompts you to either exit or cancel the Exit Command.

Edit Menu



Copy All

This menu item copies all the data to the clipboard. This data may then be pasted into other Windows applications.

Copy

This menu item copies information on one sample which has been highlighted to the clipboard. This data may then be pasted into other Windows applications, or to another sample position.

Paste

This allows you to paste sample information from the clipboard to a sample position.

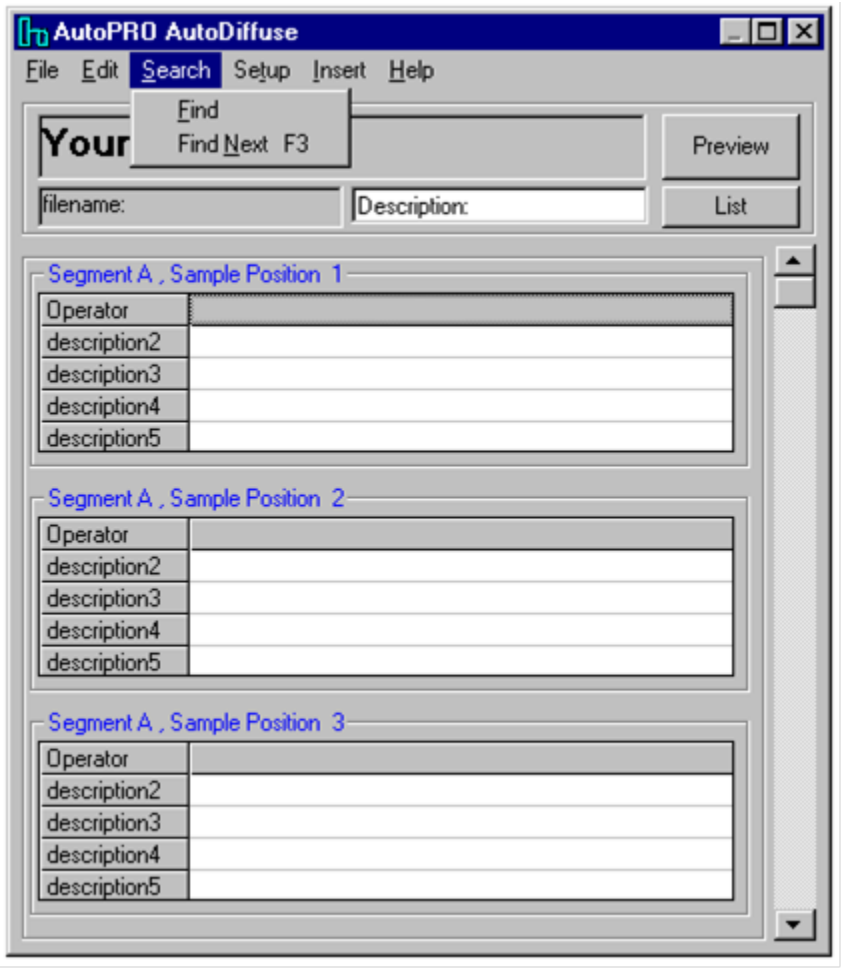
Insert

This allows you to insert a sample position. The inserted sample position is placed at the current cursor position. All following entries are moved down by one position.

Delete

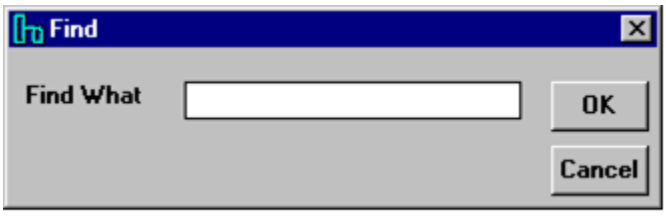
This allows you to delete a sample position. The deleted sample position is placed at the current cursor position. All following entries are moved up by one position.

Search Menu



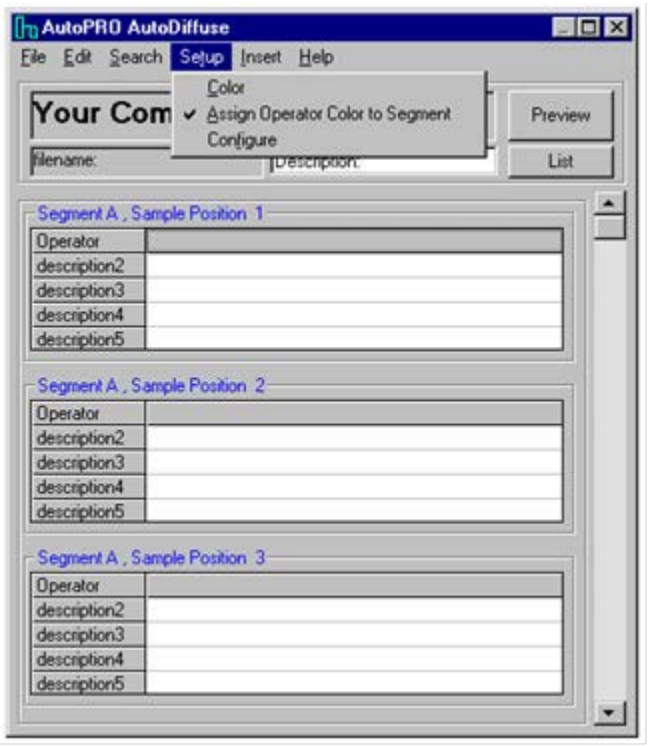
Find

On selecting this menu item, a dialog box appears. Enter the text string you wish to search for in this box. The text string will be searched for and, if present, will be highlighted.



A further occurrence of the text string entered in the find box will be searched for. If the search text is found, it will be displayed and highlighted.

Setup Menu



Color

On selecting this menu item, a dialog box appears. Enter the text string you wish to search for in this box. The text string will be searched for and, if present, will be highlighted.

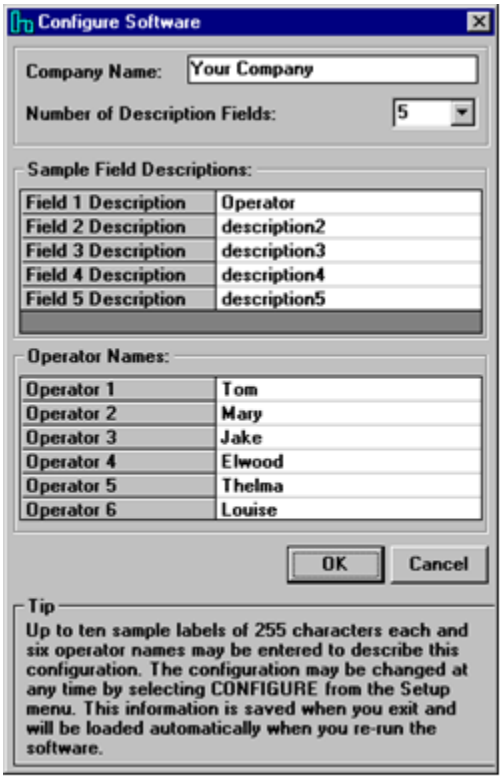
If a name is clicked, the dialog box shown below opens. This allows you to change the color assigned to the operator to a different color.

Assign Operator Color to Segment

Selecting this menu item assigns and displays the color associated with the operator. This feature is useful if several operators are using the accessory at the same time.

Configure

This menu item opens the configure dialog box. The display consists of a header area and a data area.



Company Name

Text which identifies this copy of the software is displayed here. This is usually your company name.

Number of Description Fields

The number of fields that are used to save data about the sample is set here. Up to ten fields of data may be used to identify your sample.

Sample Field Descriptions

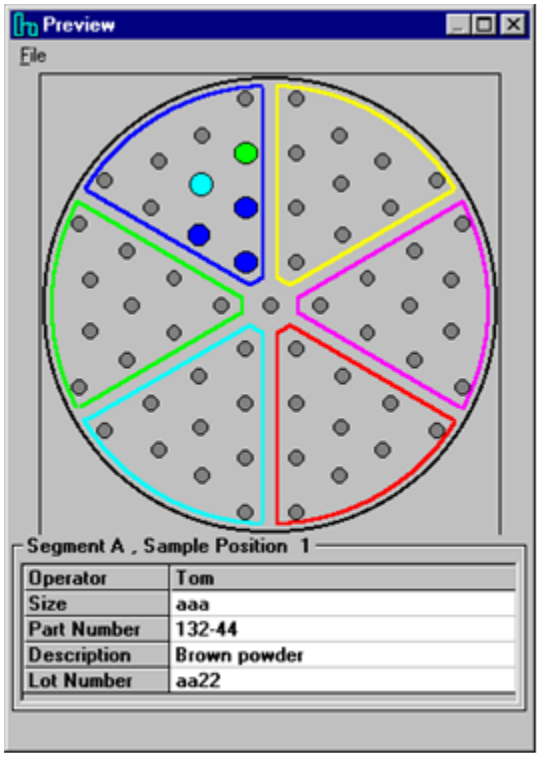
You may decide on the descriptions that you wish to use for your sample information. The first field is “hard wired” and is always Operator. The other fields should be given names that are meaningful and describe your sample, such as lot number, part number, description, etc.

Operator Names

Each segment of the sample wheel is identified by means of operator name. An operator name is not required, but sample positions will be displayed in the color selected by the operator color and it is useful to use some description to be able to identify different types of sample.

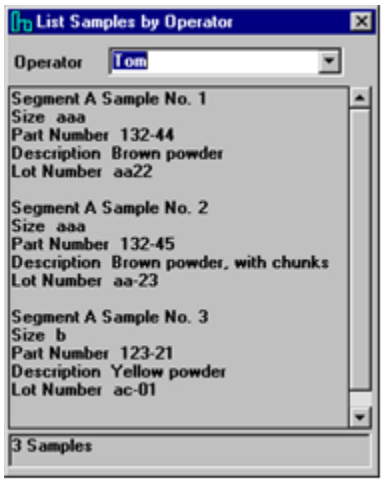
Preview

A diagram of the current AutoDiffusIR sample tray is set up with the samples in place. If a sample is present, it is shown as a colored spot, the color corresponding to the operator. By clicking on a particular sample, the information about that sample is displayed. By clicking on a sample and dragging the mouse to an empty position, the sample is moved to that position. This display is useful for final configuration of the experiment setup.



List

This button opens the list display. A list of the samples currently entered may be displayed with respect to operator. By selecting an operator name from the pull down list, the samples associated with that operator are displayed.

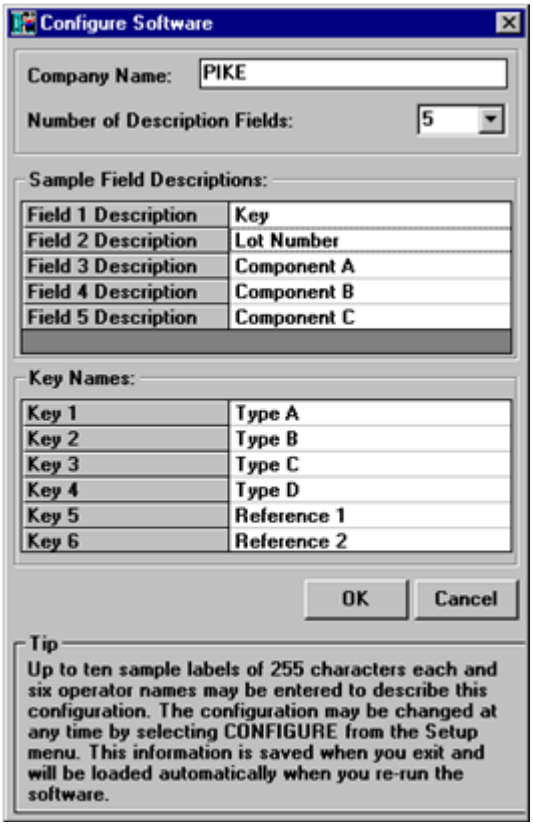


XY Stage Programmer

Introduction

The XY Stage programmer is used in conjunction with the PIKE XY Stage Accessory. This program allows the user to assign information to each sample being analyzed. Both an operator name and sampling information may be assigned to each sample in a point and click environment. The information, once entered, may be reviewed to ensure accuracy, printed out to provide a hard copy, and saved to disk in order to perform the experiment.

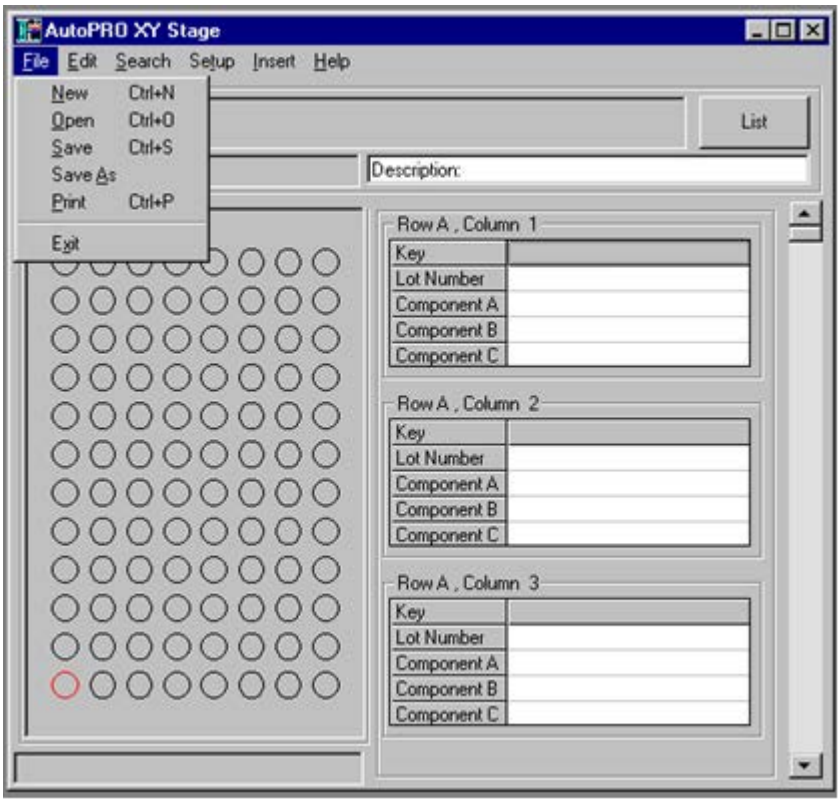
When the software is run for the first time, the configuration screen below is shown. The user may enter information to customize the software to his or her needs.



The company name may be set as well as the descriptions for the fields to be assigned to the sample. Up to six key names may also be entered.

At any time this configuration screen may be accessed by selecting configure from the setup menu.

File Menu

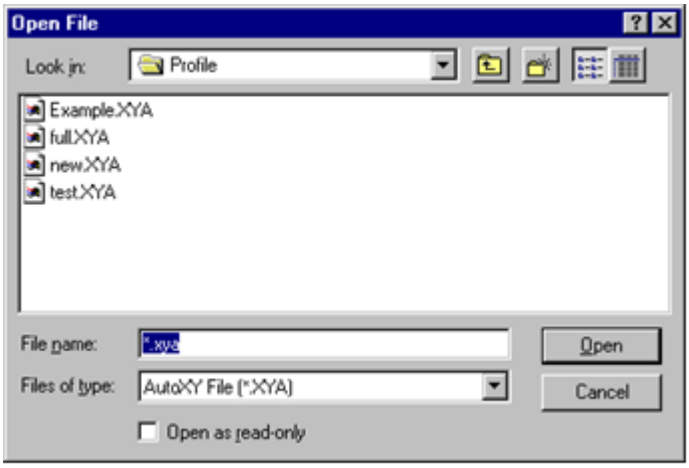


New

This command clears all data. If there are any unsaved changes when you select the New command, the software asks if you want to save the changes. The data is then cleared and the title bar is changed to [Untitled.XYA].

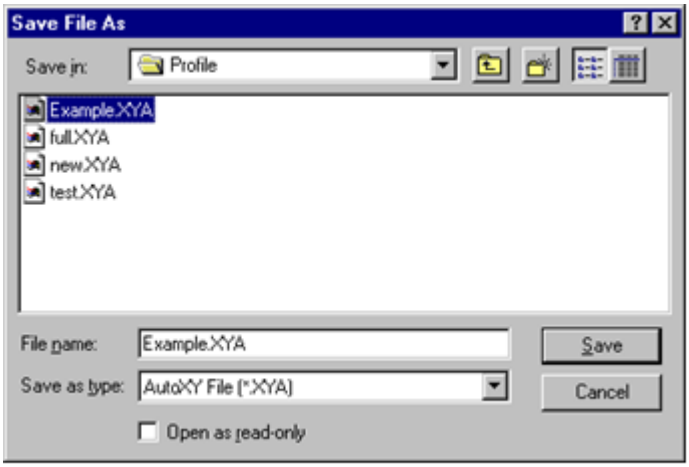
Open

This command loads a file that was previously stored on disk. The Open Dialog is displayed and you may choose the directory and file that you wish to load. Valid files have an *.XYA extension.

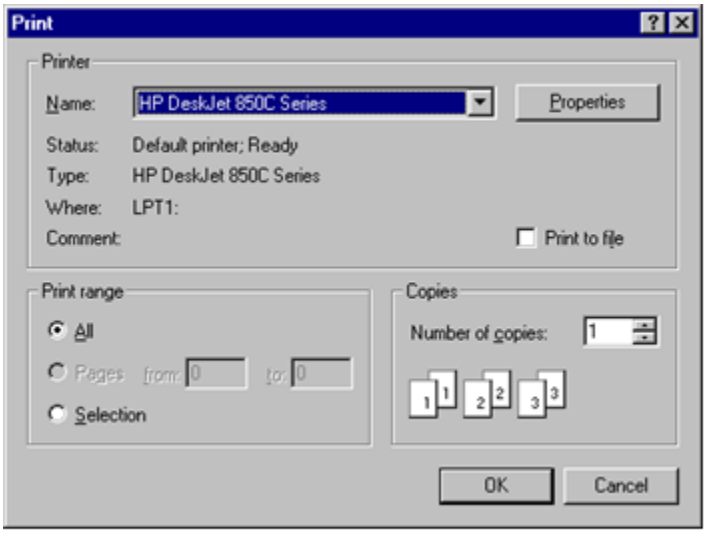


Save
This command is only enabled if a title is assigned to a file. If the file name is [Untitled.XYA] this command is not available.

Save As
This command saves your work. The **Save File As** dialog box appears so you can save the file with a different file name, or save an untitled file with a new file name.



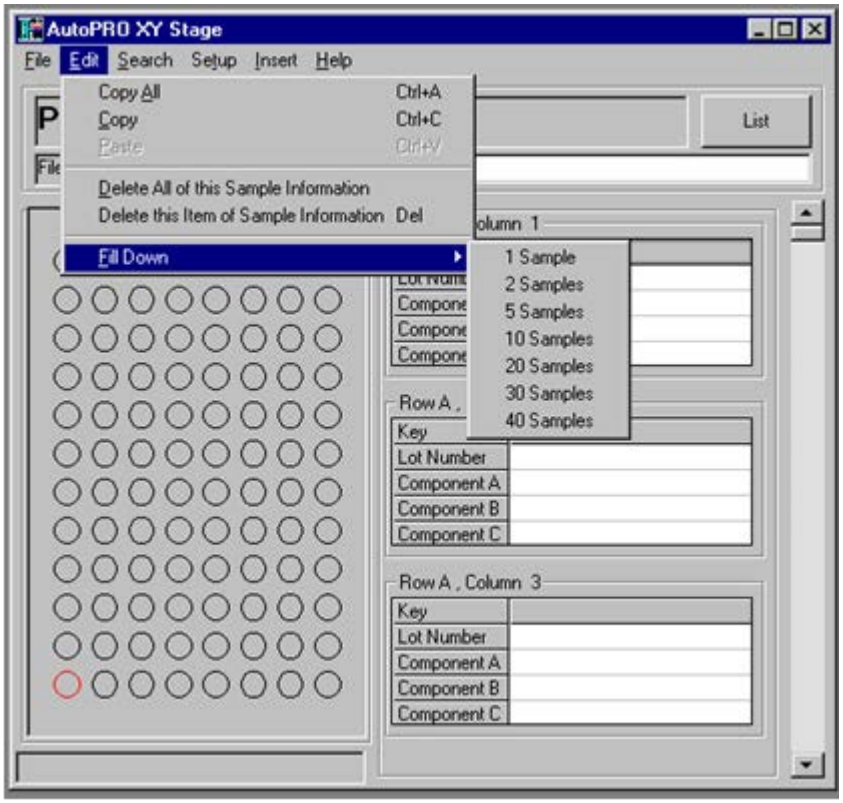
Print
This command prints the data in the data area. When selected the display below is shown.



The font type and font size may be selected prior to printing. The page to be printed may be viewed by selecting preview.

Exit
This Command closes AutoPRO. If the data has changed since your last save, AutoPRO prompts you to either exit or cancel the Exit Command.

Edit Menu



Copy All
This menu item copies all the data to the clipboard. This data may then be pasted into other Windows applications.

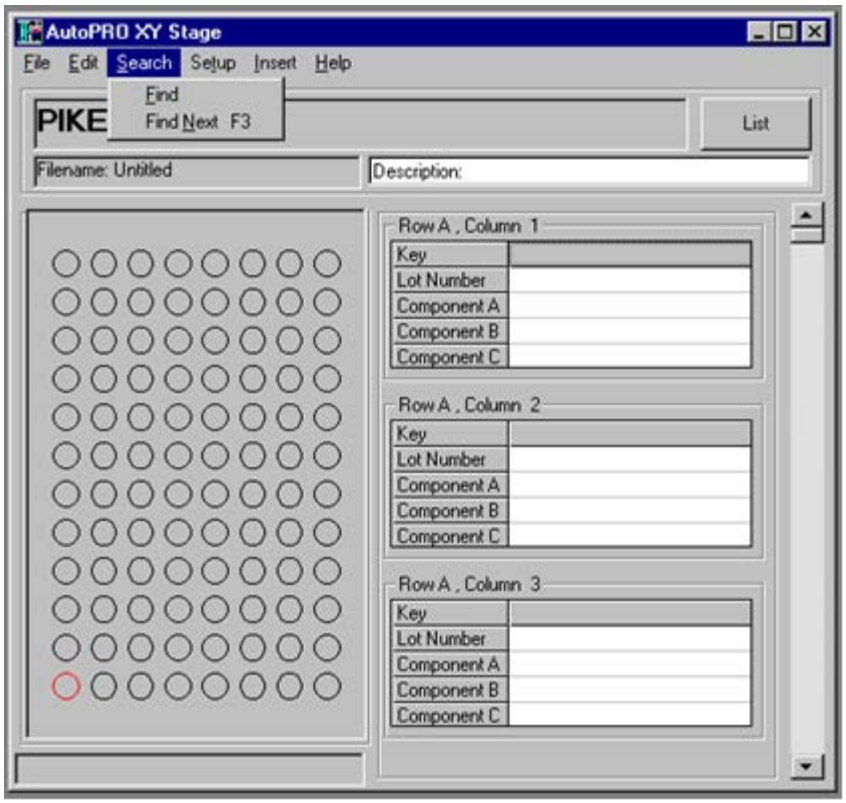
Copy
This menu item copies information on one sample which has been highlighted to the clipboard. This data may then be pasted into other Windows applications, or to another sample position.

Paste
This allows you to paste sample information from the clipboard to a sample position.

Insert
This allows you to insert a sample position. The inserted sample position is placed at the current cursor position. All following entries are moved down by one position.

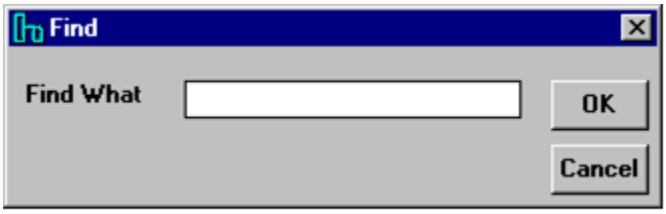
Delete
This allows you to delete a sample position. The deleted sample position is placed at the current cursor position. All following entries are moved up by one position.

Search Menu



Find

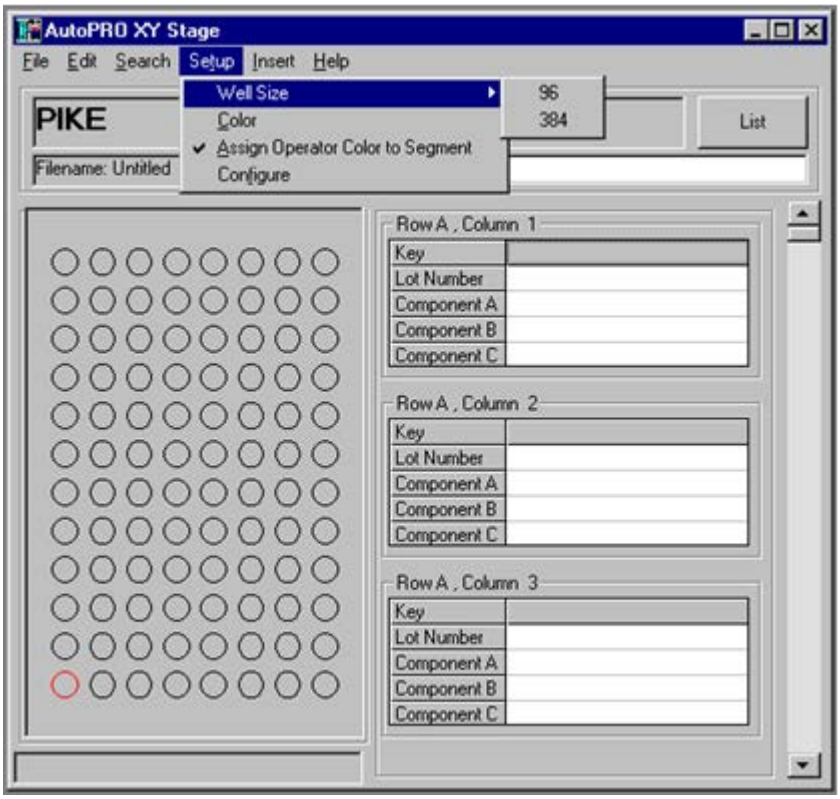
On selecting this menu item, a dialog box appears. Enter the text string you wish to search for in this box. The text string will be searched for and, if present, will be highlighted.



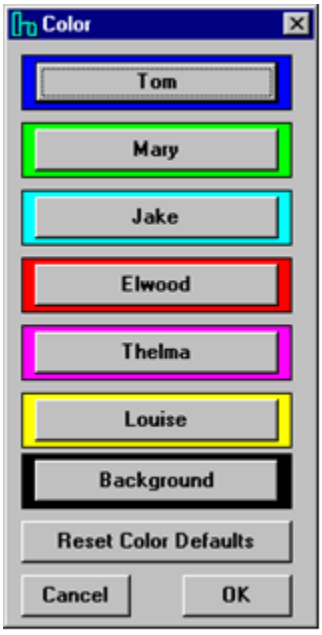
Find Next

A further occurrence of the text string entered in the find box will be searched for. If the search text is found, it will be displayed and highlighted.

Setup Menu



Color



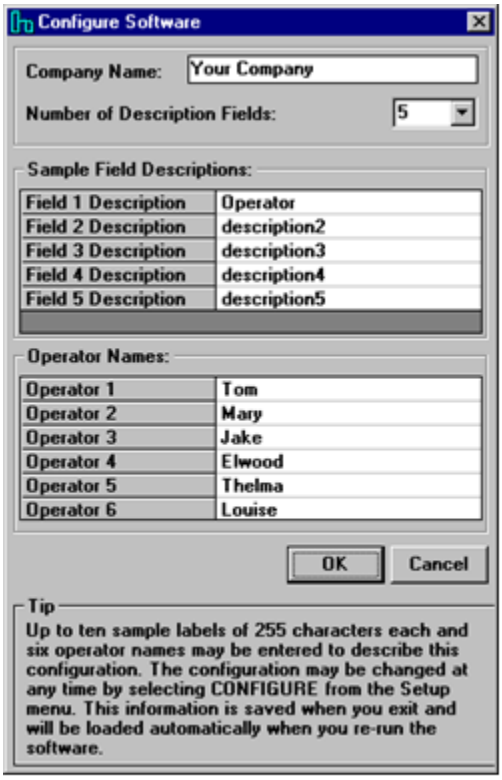
If a name is clicked, the dialog box shown below opens. This allows you to change the color assigned to the operator to a different color.

Assign Operator Color to Segment

Selecting this menu item assigns and displays the color associated with the operator. This feature is useful if several operators are using the accessory at the same time.

Configure

This menu item opens the configure dialog box. The display consists of a header area and a data area.



Company Name

Text which identifies this copy of the software is displayed here. This is usually your company name.

Number of Description Fields

The number of fields that are used to save data about the sample is set here. Up to ten fields of data may be used to identify your sample.

Sample Field Descriptions

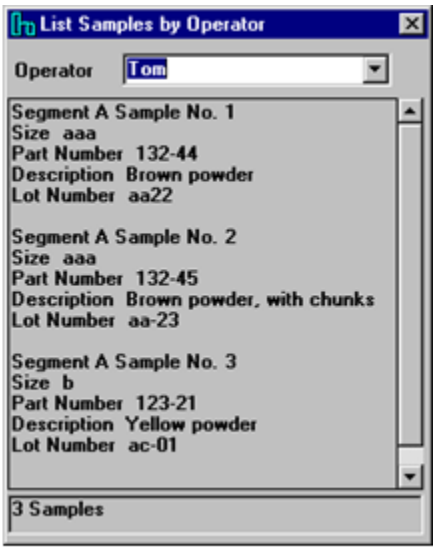
You may decide on the descriptions that you wish to use for your sample information. The first field is “hard wired” and is always Key. The other fields should be given names that are meaningful and describe your sample, such as lot number, part number, description, etc.

Key Names

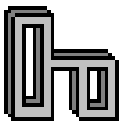
Each segment of the plate is identified by means of a key name. A Key name is not required, but sample positions will be displayed in the color selected by the Key color and it is useful to use some description to be able to identify different types of samples.

List

This button opens the list display. A list of the samples currently entered may be displayed with respect to operator. By selecting an operator name from the pull down list, the samples associated with that operator are displayed.



VeeMAX / Polarizer Programmer



Introduction

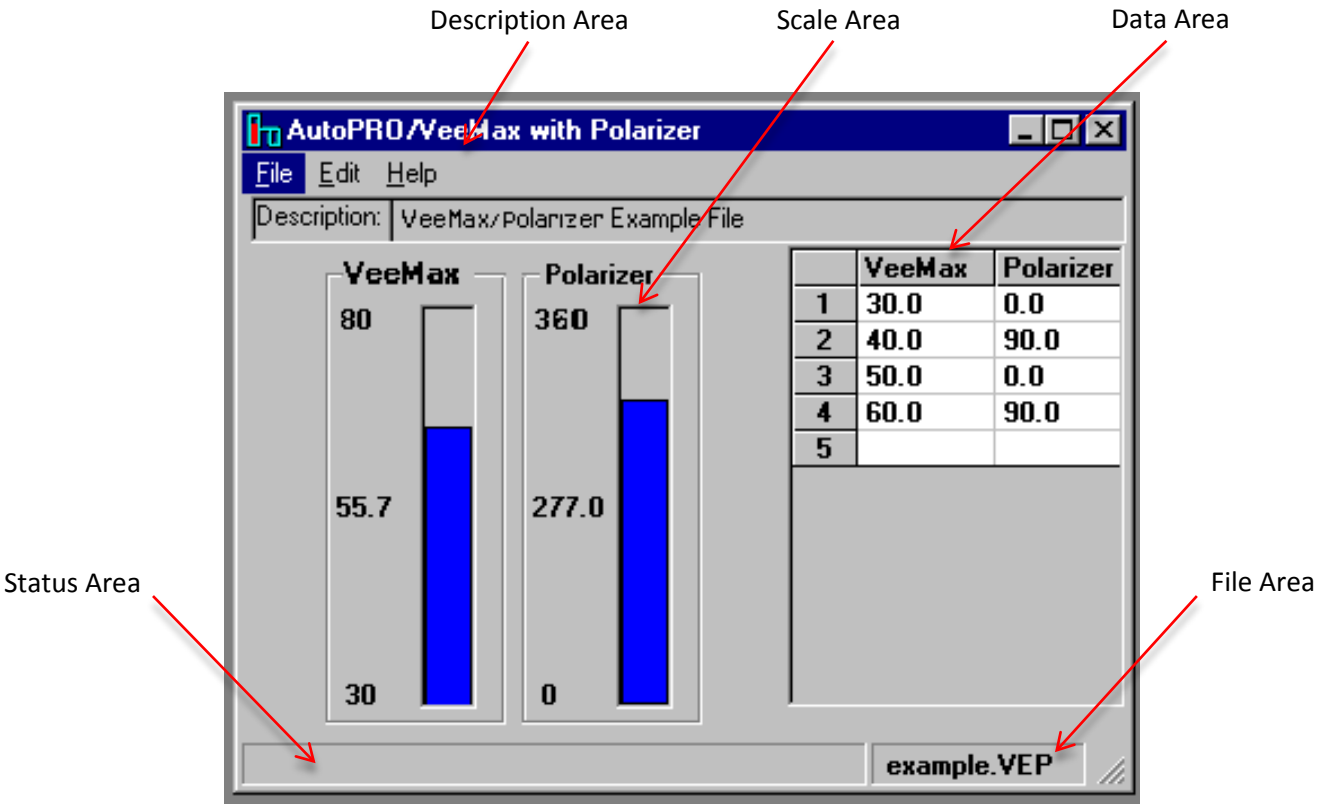
If you are operating either an automated VeeMAX or ATRMax with a polarizer, the VeeMAX/Polarizer Programmer will be displayed when you click on the program button. The operation of this program is identical for both combination accessories, except for the high and low angle limits. For these accessories, these limits are:

- VeeMAX 30° to 80°
- ATRMax 20° to 70°
- Polarizer 0° to 360°

Note that if you are using a VeeMAX/Polarizer accessory and set up AutoPRO control for an ATRMax/Polarizer accessory, although the programmer will look similar, the conversion routines to convert from angle to number of steps are different for the different accessories.

The operation of the VeeMAX/Polarizer accessory will be described here for clarity. The operation of the ATRMax/Polarizer accessory is identical.

Sections of the Display



Status Area

This area of the screen displays status information on the position of the cursor. When the cursor is in the Scale Area, the coordinates of the cursor on the scale are displayed. These numbers displayed are updated only when the cursor is in a blue portion of the scale.

Scale Area

This area of the screen displays a graphical representation of the angle of the accessory. Analysis angles may be added to the list in the Angle Area by clicking on the mouse in the **Scale Area.**

File Area

This area displays the filename of the current filename.

Data Area

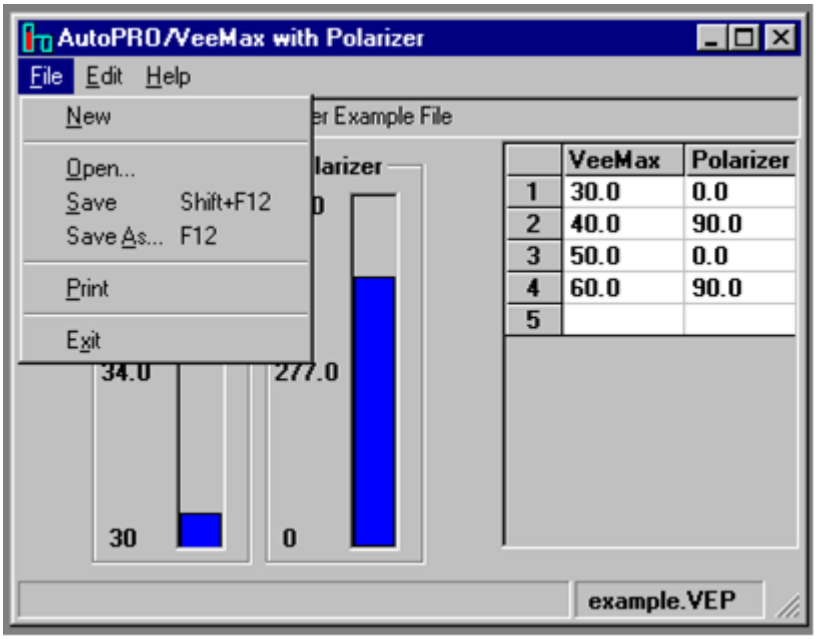
This area of the screen displays the angle to which the accessory will be moved to. The data list may be scrolled to see all the data. Points may be added to the Data Area by typing coordinates into an empty cell. Points may be deleted from the Data Area by clicking on the cell at which the change is to be made, and then selecting **Delete** from the **Edit** Menu.

Description Area

You may enter a description on the sample that you are running in this area. This description is used as the basis for automatic file generation in the AutoPRO Control program, so it is useful to enter a meaningful description here.

File Menu

This menu is used for saving and retrieving sampling configurations. The data shown on the screen may also be printed to your default Windows printer.



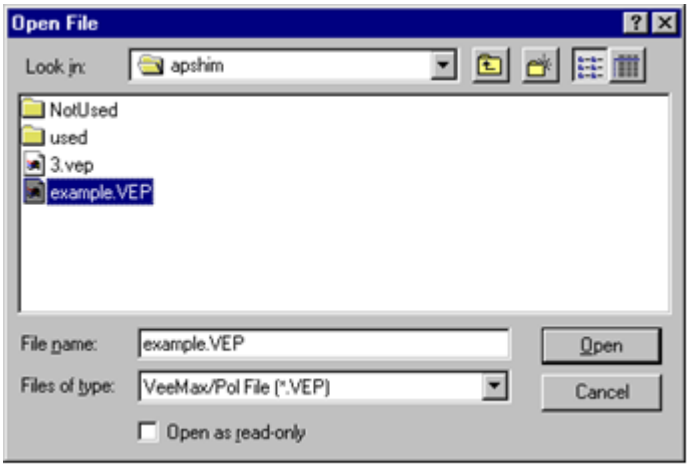
New

The **New** command clears the angle data. If there are any unsaved changes when you select the New command, AutoPRO asks if you want to save the changes. The filename is set to "Untitled.vep"

Open

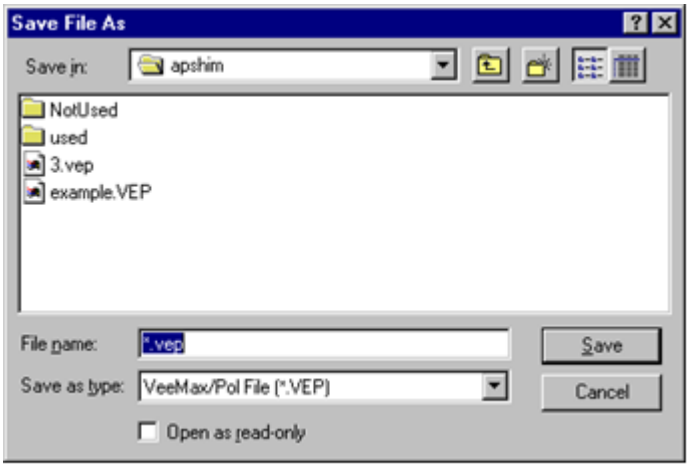
The **Open** command loads a file that was previously stored on disk. The Open Dialog is displayed and you may choose the directory and file that you wish to load. All valid files have an extension which relates to the accessory you are using.

- For VeeMAX/Polarizer, the extension is *.vep
- For ATRMax/Polarizer, the extension is *.atp



Save
The **Save** command saves your work in a file. If the File Status is clear, indicating that the file has not been named, the Save File Dialog box appears so you can give your file a name.

Save As
The **Save As** command saves your work. The Save File dialog box appears so you can save your work with a different file name.

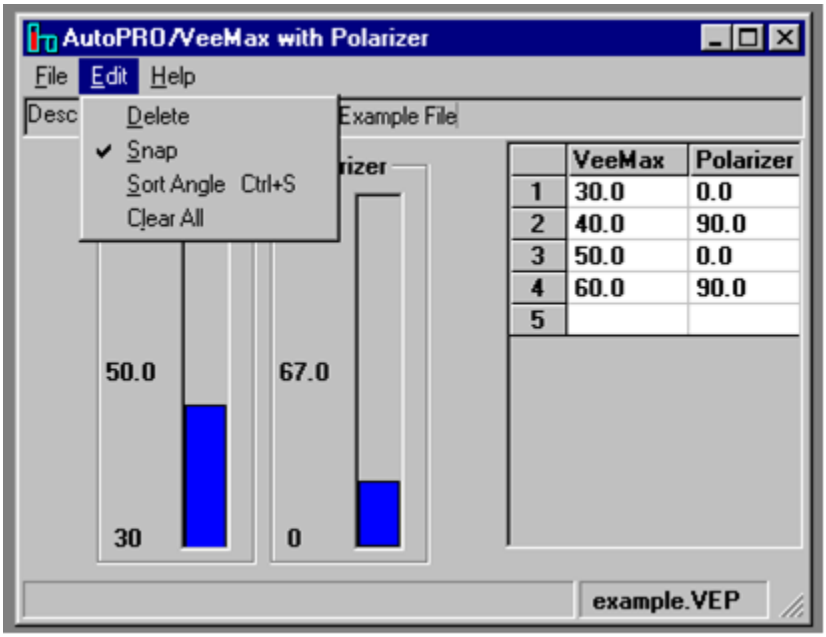


Print
The **Print** command prints a list of the data that you have entered.

Exit
The Exit Command closes AutoPRO. If the data has changed since your last save, AutoPRO prompts you to exit anyway or cancel the Exit Command.

Edit Menu

These menu items are a set of functions which are used to reorganize the data.



Delete

This command deletes a line in the angle display at the current entry point. All remaining points in the angle table are moved up one place.

Snap

When snap is selected, the entries made in the angle table due to a mouse click on the display are rounded to the nearest degree.

Sort Angle

This command allows you to reorder the points in terms of increasing angle.

Clear All

This command clears the angle data. If this data was displayed from a file, the filename will not be cleared. When changes are made after clicking on this item, they may be saved to the same filename by selecting **Save** from the File menu.

Running AutoPRO from FTIR Software

General

AutoPRO may be interfaced easily to a variety of different software packages to perform an automated analysis on your sample. In this chapter we will give examples of how this is performed for a variety of software packages. Note that in this chapter, we will use the word Macro in describing a series of commands that the FTIR software package performs. Different manufacturers use different terms for this function:

PerkinElmer	OBEY File
GRAMS	Array Basic File
Thermo	Macro
Bruker	Macro or Stored Program
Shimadzu	SBasic Program
Agilent	Script
VB/VC program	

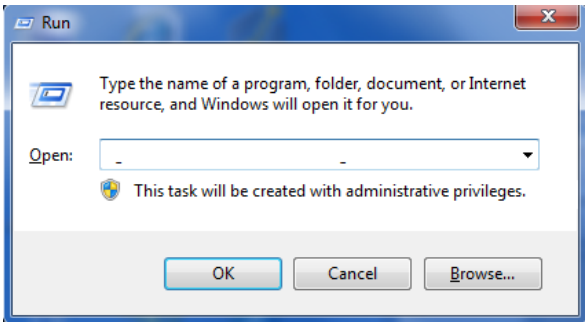
AutoPRO may be run in conjunction with other Windows based FTIR software packages. When AutoPRO is run as a separate application the accessory may be configured, programmed and controlled but it is not possible to communicate between the two software programs. To perform this communication, another software program is used called MOTOR.EXE.

MOTOR.EXE is a small program which is embedded into your FTIR Macro program in order to operate AutoPRO. Communication between MOTOR.EXE and AutoPRO is performed by means of Dynamic Data Exchange (DDE). The MOTOR program handles the details of this exchange as well as any error messages that may occur during operation, providing a simple interface to the user.

Operation

In order to illustrate the operation of MOTOR, please perform the following tutorial.

1. With Windows running, click Start and select RUN... The following dialog box will appear:



2. Click on Browse, point to your AutoPRO directory and click on MOTOR.EXE. A text string such as C:\Program Files\AutoPRO5\motor.exe will appear.

3. Click the mouse on the end of this string and enter a space and then the word Init. This last word is the command that is to be performed in AutoPRO, and is not case sensitive.

4. If you now click on the OK button, the following will happen:

    a. A small box will appear in the upper left hand corner of the display. This will contain the command that is to be transmitted to AutoPRO.

    b. AutoPRO will be opened, if it is not already running. The command, INIT, will be sent to AutoPRO and the accessory will be initialized.

So, in order to operate AutoPRO, a space, and then a command is appended to the MOTOR.EXE program Run statement. This form of command is called a "Command Line Argument". Following are several commands that may be used:

- **INIT**
  Initialize accessory. AutoPRO communicates with and sets up the Motor Controller. The accessory is then initialized to the home position.

- **UNLOAD**
  The command is used for the 6 and 8 inch wafer holder, MappIR, MAP300, Disk Checker and the AutoDiffusIR. The command moves the linear (R) stage to its furthest point so that the sample ring may be removed from the accessory. When this command has been performed, the next command must be a LOAD.

- **LOAD**
  This command loads the accessory after an unload command. The accessory is moved to its home position. If the accessory is not unloaded when this command is run, nothing happens.

- **NEWFILE filename**
  When this command is performed, the file dialog box is opened and a file containing the coordinates to be measured may be selected. If this command is followed by a filename, the dialog box is not opened to select a filename unless the filename is invalid. This allows for unattended operation of the accessory from within a Macro.

  At the completion of this command, the total number of points is saved in the file AP5.TMP which is located in your Windows directory.

- **NEXT**
  Move to the next point in a profile. If the end of the profile has been reached, nothing happens.

- **POINT n**
  The command POINT is followed by a space and a number. This is the number of the point to move to. If this number is greater than the total number of points in the profile, nothing happens.

- **DEMOON**
  Turn the demo mode on in AutoPRO

- **DEMOOFF**
  Turn the demo mode off in AutoPRO

Specific details and examples of writing macros for different FTIR packages are contained in the Appendices.

Operation without Using Command Line Arguments

Some Macro Programming languages do not support command line arguments in a call to an external (EXE) program. For this situation the following six programs have been provided in order to program your accessory:

- **INIT.EXE**
  Initialize accessory. AutoPRO communicates with and sets up the Motor Controller. The accessory is then initialized to the home position.

- **NEWFILE.EXE**
  When this command is performed, the file dialog box is opened and a file containing the coordinates to be measured may be selected.

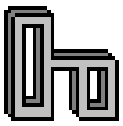
- **NEXT.EXE**
  Move to the next point in a profile. If the end of the profile has been reached, nothing happens.

- **FIRST.EXE**
  This program moves the accessory to the first point in the profile.

- **UNLOAD.EXE**
  This program unloads the accessory. The next command must be LOAD.EXE

- **LOAD.EXE**
  This program loads the accessory. The accessory is moved to its home position.

Running FTIR Software from AutoPRO



Once you have set up AutoPRO for your FTIR software, by selecting your Spectrometer type in the Setup Spectrometer Page, when you click on Background or Sample, Data will be collected.

Here we will discuss what happens when you collect data from AutoPRO, and some of the restrictions placed on this data collection by your FTIR software Macro Programming Language.

BioRad Win-IR

BioRad Win-IR uses GRAMS Array Basic as its programming language. AutoPRO communicates with Win-IR by Dynamic Data Exchange. When Win-IR is selected as the FTIR software, a program called DDE.AB is copied from the AutoPRO Directory into the Win-IR directory. DDE.AB is run when AutoPRO starts communicating with Win-IR. The Array Basic program sets up a DDE Channel with Win-IR and parses the commands sent. The following are some restrictions placed on AutoPRO by the features in Win-IR:

- **Number of Open Files**
  Win-IR has a limit on the number of spectra that may be open at any one time. These spectra are stored in slots and the maximum number of slots available is dependent on the amount of memory available, and the resolution of the data collected. If this number is exceeded, then unpredictable results may follow. In order to circumvent this problem, only one slot is used by AutoPRO. Data is collected into this window, the data is saved, and the window is closed.

- **Background Data Collection**
  Since Win-IR does not handle long filenames, the data that is collected must not be saved in a directory that has a directory name that is longer than eight characters. Background files are always collected into a file named Btmp.spc and saved into the Win-IR directory. Once this has been done, AutoPRO then copies this file into back001.spc; back002.spc etc. in the profile directory specified in AutoPRO and the current background spectral window is cleared.

- **Sample Data Collection (Using the Correct Background File)**
  When a sample spectrum is collected, it must be ratioed to a background file. Since backgrounds may be collected at all points in the profile, the correct background file has to be used. These background files are stored in the profile directory with names back001.spc, back002.spc etc. Before a sample is collected the appropriate background file is retrieved from the profile directory and renamed to BTmp.spc. The sample file is then ratioed to this background file.

- **Long Filenames**
  Long filenames are not fully supported in Win-IR. However, you may specify a long filename in AutoPRO. When AutoPRO collects a spectrum, it collects the spectrum into a file called Stmp.spc. This spectrum is stored by Win-IR in the Win-IR directory. Once the data collection is complete, the file stmp.spc is copied to the profile directory and renamed to the filename specified in AutoPRO. The collected file window is then deleted.

Background Data Collection Pseudo Code

```
If Accessory is not initialized then Initialize Accessory
If Pre-Experiment Macro defined then run Pre-Experiment Macro
Setup Background collection parameters
For i = 1 To number of background points
        Move accessory to position number i
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Background filename
        Write Background filename to C:\Windows\AP5.ini
        Write Background filename to Windows Registry
        Write Temporary Background filename to C:/Windows/AP5.ini
        Write Temporary Background filename to Windows Registry
        send resolution
        send number of background scans
        send low wavenumber limit
        send high wavenumber limit
        scan background
        Copy Background Temporary file to Background file
Next i
Closebench
```

Sample Data Collection Pseudo Code

```
If background not collected then "You must collect a background set first"
If Accessory is not initialized then Initialize Accessory
Setup Sample collection parameters
For i = 1 To Number of points in Profile
        Move Accessory to point
        If Pre-Sample Macro defined then run Pre-Sample Macro
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Sample filename
        Write Sample filename to C:\Windows\AP5.ini
        Write Sample filename to Windows Registry
        Copy Background file to BackTemp
        Set Sample temp file to Stmp.spc
        Send file format to collect
        Send number of sample scans
        Send Spectrum Comment
        Collect spectrum into SampTemp
        Save SampTemp
        Copy SampTemp to Sample Filename
        If Post-Sample Macro defined then run Post-Sample Macro
        Close file
Next i
Closebench
```

DDE.AB is an Array Basic program that is used by AutoPRO to handle the Dynamic Data Exchange and perform the commands requested. DDE.AB is general purpose in that it is used, not only for Win-IR, but for all type of Galactic GRAMS software. Because of this, there are extra commands that are parsed by DDE.AB that are not used in the Win-IR interface. The program listing of DDE.AB is shown at the end of this chapter.

Bomem GRAMS

Bomem GRAMS uses GRAMS Array Basic as its programming language. AutoPRO communicates with Bomem GRAMS by Dynamic Data Exchange. When Bomem GRAMS is selected as the FTIR software, a program called DDE.AB is copied from the AutoPRO Directory into the Bomem GRAMS directory. DDE.AB is run when AutoPRO starts communicating with Bomem GRAMS. The Array Basic program sets up a DDE Channel with Bomem GRAMS and parses the commands sent. The following are some restrictions placed on AutoPRO by the features in Bomem GRAMS:

- **Number of Open Files**
  Bomem GRAMS has a limit on the number of spectra that may be open at any one time. These spectra are stored in slots and the maximum number of slots available is dependent on the amount of memory available, and the resolution of the data collected. If this number is exceeded, then unpredictable results may follow. In order to circumvent this problem, only one slot is used by AutoPRO. Data is collected into this window, the data is saved, and the window is closed.

- **Background Data Collection**
  Since Bomem GRAMS does not handle long filenames, the data that is collected must not be saved in a directory that has a directory name that is longer than eight characters in length. Background files are always collected into a file named Btmp.spc and saved into the Bomem GRAMS directory. Once this has been done, AutoPRO then copies this file into back001.spc; back002.spc etc. in the profile directory specified in AutoPRO and the current background spectral window is cleared.

- **Sample Data Collection (Using the Correct Background File)**
  When a sample spectrum is collected, it must be ratioed to a background file. Since backgrounds may be collected at all points in the profile, the correct background file has to be used. These background files are stored in the profile directory with names back001.spc, back002.spc etc. Before a sample is collected the appropriate background file is retrieved from the profile directory and renamed to BTmp.spc. The sample file is then ratioed to this background file.

- **Long Filenames**
  Long filenames are not fully supported in Bomem GRAMS. However, you may specify a long filename in AutoPRO. When AutoPRO collects a spectrum, it collects the spectrum into a file called Stmp.spc. This spectrum is stored by Bomem GRAMS in the Bomem GRAMS directory. Once the data collection is complete, the file Stmp.spc is copied to the profile directory and renamed to the filename specified in AutoPRO. The collected file window is then deleted.

Background Data Collection Pseudo Code

```
If Accessory is not initialized then Initialize Accessory
If Pre-Experiment Macro defined then run Pre-Experiment Macro
Setup Background collection parameters
For i = 1 To number of background points
        Move accessory to position number i
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Background filename
        Write Background filename to C:\Windows\AP5.ini
        Write Background filename to Windows Registry
        Write Temporary Background filename to C:/Windows/AP5.ini
        Write Temporary Background filename to Windows Registry
        send number of background scans
        send low wavenumber limit
        send high wavenumber limit
        scan background
        Copy Background Temporary file to Background file
Next i
Closebench
```

Sample Data Collection Pseudo Code

```
If background not collected then "You must collect a background set first"
If Accessory is not initialized then Initialize Accessory
Setup Sample collection parameters
For i = 1 To Number of points in Profile
        Move Accessory to point
        If Pre-Sample Macro defined then run Pre-Sample Macro
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Sample Filename
        Write Sample filename to C:\Windows\AP5.ini
        Write Sample filename to Windows Registry
        Copy Background file to BackTemp
        Set Sample Temp File to Stmp.spc
        Send file format to collect
        Send number of sample scans
        Send Spectrum Comment
        Collect spectrum into SampTemp
        Save SampTemp
        Copy SampTemp to Sample Filename
        If Post-Sample Macro defined then run Post-Sample Macro
        Close file
Next i
Closebench
```

DDE.AB is an Array Basic program that is used by AutoPRO to handle the Dynamic Data Exchange and perform the commands requested. DDE.AB is general purpose in that it is used, not only for Bomem GRAMS, but for all type of Galactic GRAMS software. Because of this, there are extra commands that are parsed by DDE.AB that are not used in the Bomem GRAMS interface.

Midac GRAMS

Midac GRAMS uses GRAMS Array Basic as its programming language. AutoPRO communicates with Midac GRAMS by Dynamic Data Exchange. When Midac GRAMS is selected as the FTIR software, a program called DDE.AB is copied from the AutoPRO Directory into the Midac GRAMS directory. DDE.AB is run when AutoPRO starts communicating with Midac GRAMS. The Array Basic program sets up a DDE Channel with Midac GRAMS and parses the commands sent. The following are some restrictions placed on AutoPRO by the features in Midac GRAMS:

- **Number of Open Files**
  Midac GRAMS has a limit on the number of spectra that may be open at any one time. These spectra are stored in slots and the maximum number of slots available is dependent on the amount of memory available, and the resolution of the data collected. If this number is exceeded, then unpredictable results may follow. In order to circumvent this problem, only one slot is used by AutoPRO. Data is collected into this window, the data is saved, and the window is closed.

- **Background Data Collection**
  Since Midac GRAMS does not handle long filenames, the data that is collected must not be saved in a directory that has a directory name that is longer than eight characters. Background files are always collected into a file named Btmp.spc and saved into the Midac GRAMS directory. Once this has been done, AutoPRO then copies this file into back001.spc, back002.spc etc. in the profile directory specified in AutoPRO. Once this has been done, the current background spectral window is cleared.

- **Sample Data Collection (Using the Correct Background File)**
  When a sample spectrum is collected, it must be ratioed to a background file. Since backgrounds may be collected at all points in the profile, the correct background file has to be used. These background files are stored in the profile directory with names back001.spc, back002.spc etc. Before a sample is collected the appropriate background file is retrieved from the profile directory and renamed to BTmp.spc. The sample file is then ratioed to this background file.

- **Long Filenames**
  Long filenames are not fully supported in Midac GRAMS. However, you may specify a long filename in AutoPRO. When AutoPRO collects a spectrum, it collects the spectrum into a file called Stmp.spc. This spectrum is stored by Midac GRAMS in the Midac GRAMS directory. Once the data collection is complete, the file Stmp.spc is copied to the profile directory and renamed to the filename specified in AutoPRO. The collected file window is then deleted.

Background Data Collection Pseudo Code

```
If Accessory is not initialized then Initialize Accessory
If Pre-Experiment Macro defined then run Pre-Experiment Macro
Setup Background collection parameters
For i = 1 To number of background points
        Move accessory to position number i
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Background filename
        Write Background filename to C:\Windows\AP5.ini
        Write Background filename to Windows Registry
        Write Temporary Background filename to C:/Windows/AP5.ini
        Write Temporary Background filename to Windows Registry
        send resolution
        send number of background scans
        send low wavenumber limit
        send high wavenumber limit
        scan background
        Copy Background Temporary file to Background file
Next i
Closebench
```

Sample Data Collection Pseudo Code

```
If background not collected then "You must collect a background set first"
If Accessory is not initialized then Initialize Accessory
Setup Sample collection parameters
For i = 1 To Number of points in Profile
        Move Accessory to point
        If Pre-Sample Macro defined then run Pre-Sample Macro
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Sample filename
        Write Sample filename to C:\Windows\AP5.ini
        Write Sample filename to Windows Registry
        Copy Background file to BackTemp
        Set Sample temp file to Stmp.spc
        Send file format to collect
        Send number of sample scans
        Send Spectrum Comment
        Collect spectrum into SampTemp
        Save SampTemp
        Copy SampTemp to Sample Filename
        If Post-Sample Macro defined then run Post-Sample Macro
        Close file
Next i
Closebench
```

DDE.AB is an Array Basic program that is used by AutoPRO to handle the Dynamic Data Exchange and perform the commands requested. DDE.AB is general purpose in that it is used, not only for Midac GRAMS, but for all type of Galactic GRAMS software. Because of this, there are extra commands that are parsed by DDE.AB that are not used in the Midac GRAMS interface.

Mattson WinFIRst

Mattson WinFIRst uses Mattson ApPro as its programming language.

Nicolet OMNIC

Nicolet OMNIC has two Macro programming systems; MACROS/Basic and MACROS/Pro. AutoPRO communicates with OMNIC using the Macros/Pro language.

Background Data Collection

```
If Accessory is not initialized then Initialize Accessory
If Pre-Experiment Macro defined then run Pre-Experiment Macro
set resolution
set number of background scans
set low wavenumber limit
set high wavenumber limit
For i = 1 To number of background points
        Move accessory to position number i
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Background filename
        Write Background filename to C:\Windows\AP5.ini
        Write Background filename to Windows Registry
        Collect Background
        Save Background file
        Delete Spectrum
        Close file
Next i
```

Sample Data Collection

```
If background not collected then "You must collect a background set first"
If Accessory is not initialized then Initialize Accessory
Set file format to collect
Set number of sample scans
For i = 1 To Number of points in Profile
        Move Accessory to point
        If Pre-Sample Macro defined then run Pre-Sample Macro
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Sample filename
        Write Sample filename to C:\Windows\AP5.ini
        Write Sample filename to Windows Registry
        Collect Sample file
        Add Sample Information to Spectrum Comment
        Save Sample file
        If Post-Sample Macro defined then run Post-Sample Macro
        Delete Spectrum
Next i
Closebench
```

Shimadzu Hyper-IR

Hyper-IR has a built in macro programming language called SBasic. If SBasic is not available on your copy of Hyper-IR, you should contact Shimadzu for installation of this feature.

AutoPRO communicates with Hyper-IR using Dynamic Data Exchange, and the features found in SBasic. The following are some restrictions placed on AutoPRO by the features in Hyper-IR:

- **Number of Open Files**
  Hyper-IR has a limit on the number of spectral windows that may be open at any one time. If this number is exceeded, then unpredictable results may follow. In order to circumvent this problem, only one spectral window is used by AutoPRO. Data is collected into this window, the data is saved, and the window is closed.

- **Background Data Collection**
  Since Hyper-IR does not handle long filenames, the data that is collected must not be saved in a directory that has a directory name that is longer than eight characters in length. Background files are always collected into a file named Btmp.irs and saved into the Hyper-IR directory. Once this has been done, AutoPRO then copies this file into back001.irs; back002.irs etc. in the profile directory specified in AutoPRO and the current background spectral window is cleared.

- **Sample Data Collection (Using the Correct Background File)**
  When a sample spectrum is collected, it must be ratioed to a background file. Since backgrounds may be collected at all points in the profile, the correct background file has to be used. Hyper-IR uses a specially named background file to ratio a sample spectrum to. The name of this background file is dependent on the resolution of the data being collected.

Resolution cm^{-1}	Background Filename
1	c:\windows\specsys\ss80d100.bkg
2	c:\windows\specsys\ss80d200.bkg
4	c:\windows\specsys\ss80d400.bkg
8	c:\windows\specsys\ss80d800.bkg
16	c:\windows\specsys\ss80d016.bkg

- **Long Filenames**
  Long filenames are not fully supported in Hyper-IR. However, you may specify a long filename in AutoPRO. When AutoPRO collects a spectrum, it collects the spectrum into a file called Stmp.irs. This spectrum is stored by Hyper-IR in the Hyper-IR directory. Once the data collection is complete, the file Stmp.irs is copied to the profile directory and renamed to the filename specified in AutoPRO. The collected file window is then deleted.

The spectrum that is collected has to be ratioed to its correct background file. Background files are always sequentially named back001.irs, back002.irs etc. Before collecting a sample spectrum, the correct background file, Back001.irs, Back002.irs etc. is copied into the correct background file in the c:\windows\specsys\ directory.

Background Data Collection Pseudo Code

```
If Accessory is not initialized then Initialize Accessory
If Pre-Experiment Macro defined then run Pre-Experiment Macro
Setup Background collection parameters
For i = 1 To number of background points
        Move accessory to position number i
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Background filename
        Write Background filename to C:\Windows\AP5.ini
        Write Background filename to Windows Registry
        Select Case resolution
                Case 1
                BackTemp = "c:\windows\specsys\ss80d100.bkg"
                Case 2
                BackTemp = "c:\windows\specsys\ss80d200.bkg"
                Case 4
                BackTemp = "c:\windows\specsys\ss80d400.bkg"
                Case 8
                BackTemp = "c:\windows\specsys\ss80d800.bkg"
                Case 16
                BackTemp = "c:\windows\specsys\ss80d016.bkg"
        End Select
        Write Temporary Background filename to C:/Windows/AP5.ini
        Write Temporary Background filename to Windows Registry
        send resolution
        send number of background scans
        send low wavenumber limit
        send high wavenumber limit
        scan background
        Copy Background Temporary file to Background file
Next i
Closebench
```

Sample Data Collection Pseudo Code

```
If background not collected then "You must collect a background set first"
If Accessory is not initialized then Initialize Accessory
Setup Sample collection parameters
For i = 1 To Number of points in Profile
        Move Accessory to point
        If Pre-Sample Macro defined then run Pre-Sample Macro
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Sample filename
        Write Sample filename to C:\Windows\AP5.ini
        Write Sample filename to Windows Registry
        Select Case res
```

```
                Case 1
                BackTemp = "c:\windows\specsys\ss80d100.bkg"
                Case 2
                BackTemp = "c:\windows\specsys\ss80d200.bkg"
                Case 4
                BackTemp = "c:\windows\specsys\ss80d400.bkg"
                Case 8
                BackTemp = "c:\windows\specsys\ss80d800.bkg"
                Case 16
                BackTemp = "c:\windows\specsys\ss80d016.bkg"
        End Select
        Copy Background file to BackTemp
        Set Sample Temp File to Stmp.irs
        Send file format to collect
        Send number of sample scans
        Send Spectrum Comment
        Collect spectrum into SampTemp
        Save SampTemp
        Copy SampTemp to Sample Filename
        If Post-Sample Macro defined then run Post-Sample Macro
        Close file
Next i
Closebench
```

PerkinElmer Spectrum

PerkinElmer Spectrum v5.x uses the OBEY programming system, which is based on Visual Basic. AutoPRO5.0 is written using 32 bit code, whereas OBEY is a 16 bit language only. Because of this, the OBEY software code cannot be embedded into AutoPRO5.0. When PerkinElmer Spectrum is chosen as your FTIR software, an OBEY program called APPE.exe is used to collect the FTIR data. Communication to APPE.exe is by means of Dynamic Data Exchange.

APPE.exe has four valid commands. These are:

1. **Init**
   Initialize sets up the OBEY Program to initialize the spectrometer and set basic parameters.

2. **Back**
   When this command is sent to APPE.exe, the program checks the AP5.ini file to find out the current values of resolution, wavenumber limits, number of background scans, and filename to save as. A background spectrum is collected with these parameters and saved to the spectra directory.

3. **Sample**
   When this command is sent to APPE.exe, the program checks the AP5.ini file to find out the current value of the number of sample scans and the final file format desired. A sample spectrum is collected with these parameters and saved to the spectra directory.

4. **Close**
   This command closes OBEY and the APPE.exe program.

The following are some restrictions placed on AutoPRO by the features in the OBEY-programming language:

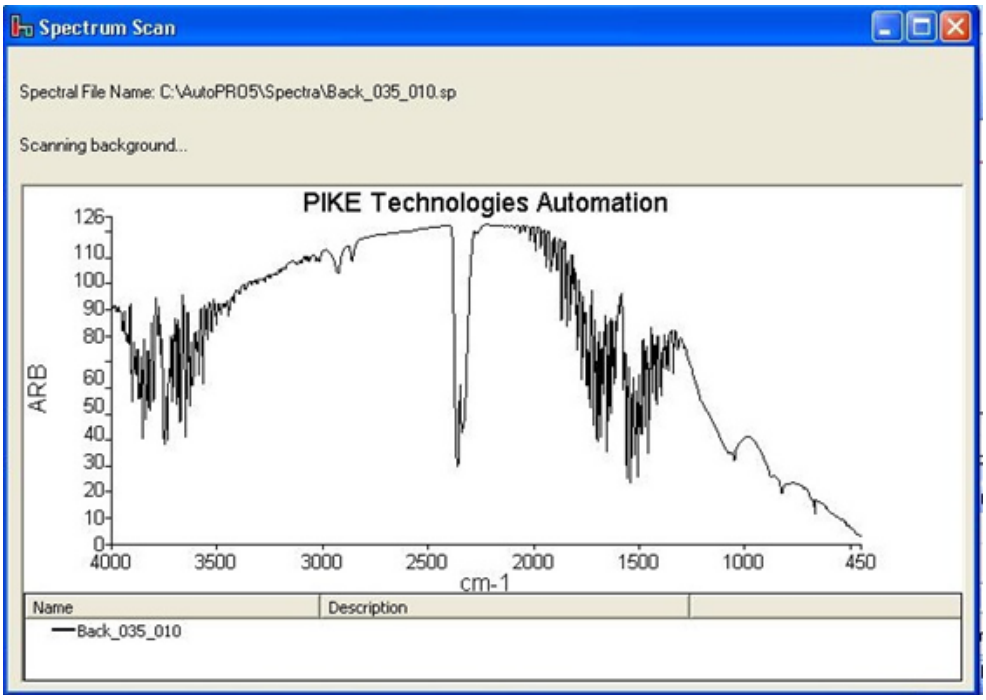
- **Stored Background Files**
  When collecting spectra in OBEY, there is no capability for using a background file that has been stored to a disk. There are several automated accessories that must use stored background files. In order to circumvent this restriction, when a spectrum has to be ratioed to a stored background, the spectrum is collected as a single beam spectrum. This spectrum is then ratioed to the stored background file, and then saved to disk.

- **Long Filenames**
  The 16 bit OBEY programming language is not capable of handling either long filenames or long directory names. In many cases, AutoPRO will be installed in a directory below Program Files. This directory has a long filename and so spectra cannot be directly saved into the AutoPRO directory. Similarly OBEY cannot handle backgrounds stored in a long directory name location or with long filenames.

  To circumvent this restriction, background files are collected into a file named BTmp.sp, and stored in the Spectrum directory. Once the data collection is complete, and control is returned to AutoPRO, this file is copied into the directory specified by the AutoPRO default Spectral Directory with the filename Back001.sp, back002.sp etc.

PerkinElmer Spectrum v6.x and 10.x

When AutoPro is configured for PerkinElmer Spectrum software versions 6.x and 10.x a separate window is opened when data collection is initiated. An example of the window is:



NOTE: It is recommended that the data collection parameters be set up in the Spectrum Software prior to collecting data with AutoPRO. AutoPRO will use the existing parameters during data collection.

This window will display the live single beam as it is being collected at each specified point in the profile. The resulting spectra will be saved in the default Spectral Save directory (refer to page 19).

Sample files are collected as single beam spectral. They are then ratioed to the correct background file if required. Each sample file is stored with the filename Stmp.sp in the Spectrum directory. Once the data collection is complete, and control is returned to AutoPRO, this file is copied into the directory specified by the AutoPRO default Spectral Directory, and with the filename specified by the user.

Background Data Collection Pseudo Code

```
If Accessory is not initialized then Initialize Accessory
If Pre-Experiment Macro defined then run Pre-Experiment Macro
        Launch appe.exe
For i = 1 To number of background points
        Move accessory to position number i
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Background filename
        Write Background filename to C:\Windows\AP5.ini
        Write Background filename to Windows Registry
        Write Temporary Background filename to C:/Windows/AP5.ini
        Write Temporary Background filename to Windows Registry
        Write Background Collection parameters to AP5.ini
        Transmit INIT to APPE.exe
        Transmit Back to APPE.exe
        Copy Background Temporary file to Background file
Next i
Closebench
```

Sample Data Collection Pseudo Code

```
If background not collected then "You must collect a background set first"
If Accessory is not initialized then Initialize Accessory
For i = 1 To Number of points in Profile
        Move Accessory to point
        If Pre-Sample Macro defined then run Pre-Sample Macro
        Save Data Collection Settings to Windows Registry
        Save Data Collection Settings to C:\Windows\AP5.ini
        Create Sample filename
        Write Sample filename to C:\Windows\AP5.ini
        Write Sample filename to Windows Registry
        Copy Background file to BackTemp
        Set Sample Temp File to Stmp.spc
        Send file format to collect
        Send number of sample scans
        WITHIN APPE.EXE
                Collect single beam scan to Stmp.sp
                If final format=transmission, ratio Stmp.sp to Btmp.sp
                If final format = absorbance, convert ratioed spectrum to Absorbance
                Send Spectrum Comment
                Save Sample spectrum to Stmp.sp
        Copy SampTemp to Sample Filename
        If Post-Sample Macro defined then run Post-Sample Macro
        Close file
Next i
Closebench
```

BioRad Win-IR PRO/Merlin

BioRad Win IR PRO and Merlin utilize the Bio-Rad scripting language as its macro programming language.

DDE.AB Program Listing

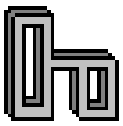
```
troff
'*********************************************************
'       The DDE string $arg is the correct syntax to
'       use in the DRIVER command.
'       Check for Scan keyword and run driver statement
'
'       MRU:  9/5/97 dje
'       added code for Midac/Bomem instruments ver 3.02 driver ver 1.06
'       MRU:    2/22/99 prb
'       added code for MACRO command
'*********************************************************
'initialize variables
        free
        free arg : dim arg(120)
        free cmd : dim cmd(120)
        free cmd2 : dim cmd2(5)
        free errcode : dim errcode(64)
        free valcmd1  : dim valcmd1(5)
        free valcmd2  : dim valcmd2(5)
        free valcmd3  : dim valcmd3(5)
        free valcmd4  : dim valcmd4(5)
        free valcmd5  : dim valcmd5(5)
        free valcmd6  : dim valcmd6(5)
        free valcmd7  : dim valcmd7(5)
        free valcmd8  : dim valcmd8(5)
        free valcmd9  : dim valcmd9(5)
        free npart : dim npart(15)
        free iputarg : dim iputarg(64)
        free fname    : dim fname(128)

        string $valcmd1 = "Scan"
        string $valcmd2 = "WAIT"
        string $valcmd3 = "ISCAN"
        string $valcmd4 = "RES"
        string $valcmd5 = "NSCAN"
        string $valcmd6 = "IPUT"
        string $valcmd7 = "ABS"
        string $valcmd8 = "TRANS"
        string $valcmd9 = "MACRO"
```

```
'  ******  for testing only comment out ddelink and remove comment from string $arg

        ddelink #0,9,"$arg"
        'string $arg="MACRO c:\win-ir\fileinfo.ab"

'parse data from dde string
        for i=0 to 120
                cmd(i)=arg(i)
        next i

'check command and jump to command handler
'cannot compare strings using if statement so
'compare spelling of command with valid command


    ' ABS Command
        if cmd(0,2)<> valcmd7(0,2) then goto 390
        driver "IPUT YTYPE",2
        goto 600

390   ' TRANS Command
        if cmd(0,4)<> valcmd8(0,4) then goto 400
        driver "IPUT YTYPE",128
        goto 600

400   ' WAIT command
        if cmd(0,3) <> valcmd2(0,3) then goto 420
        Driver "IPUT WAIT",1:troff
        goto 600

420     ' RES command
        if cmd(0,2) <> valcmd4(0,2) then goto 460
        for i=0 to 3
        if cmd(4+i)=120 then i=4: goto 430 'term char "x"
                npart(i)=cmd(4+i)                       'form new string
430     next i
        string npart,-20            'convert string to number
        resval=v
```

```
        driver "IPUT RES",resval
        goto 60

        ' Scan command
460     if cmd(0,4) <> valcmd5(0,4) then goto 490
        for i=0 to 5
        if cmd(6+i)=120 then i=6: goto 470          'term char "x"
                npart(i)=cmd(6+i)                   'form new string
470     next i
        string npart,-20            'convert string to number
        scanval=v
        driver "IPUT SCANS",scanval
        goto 600

490     ' IPUT command
        if cmd(1,3) <> valcmd6(1,3) then  goto 550
        iputarg(0,3)=arg(5,8)
        if iputarg(0)=66 then goto 520  'if 1st letter (B)eam
        nameend=index0(arg)
        'get end of pathname and set fname to full path
        string $fname(0,nameend-11)=$arg(11,nameend)
        Driver "iput name",$fname
        goto 600

520     'beam argument
        if arg(11)=98 then goto 540         'if first letter (b)kg
        driver "IPUT BEAM","SAMPLE"
        goto 600
540     driver "IPUT BEAM","BACKGROUND"
        goto 600

550     'Scan Command
        if cmd(0,3) <> valcmd1(0,3) then goto 560
555     if getsfile() <> 0  then setfile 1 :  noshow : goto 555  'clear all slots
        ONPAINT 0:SEE

        Driver $arg
        goto 600

560     ' ISCAN command
```

```
'start at 2nd letter, gets fooled if 1st letters are same
        if cmd(0,4) <> valcmd3(0,4) then goto 580
570     if getsfile() <> 0  then setfile 1 :  noshow : goto 570  'clear all slots
        ONPAINT 0:SEE

        Driver "iscan"
        goto 600

580     ' MACRO command
                if cmd(0,4) <> valcmd9(0,4) then goto 590          'valid command not
                found. go to error handler
        'get end of pathname and set fname to full path
        nameend=index0(arg)
        string $fname=$arg(6,nameend)
        ' now call the program and wait til it is finished
        doprogram $fname

'dialogon
'print
'!beep
'print "Debugging example message"
'print
'dialogoff

        goto 600          'have a valid command at index j
590     string $errcode = "9999"          'Set error code
                goto 10090                'no valid commands, exit program with wrong
                                          command errorcode

600     'we have a valid command
        onerror -1
        string $errcode="0"
        goto 10090


10050   'set up error code and return
        string errcode , -19

10090   ddelink #0,8,"$errcode"
10100   end
```

File Structures



During operation, AutoPRO writes several files to disk, as follows.

Profile Files

These are the files that are written by the programmers, and contain information about the points to be analyzed. There are four types of profile files written by the programmers.

VeeMAX, ATRMax, Polarizer, RotatIR

These four programmers share the same profile file structure. Each programmer saves the profile with its own extension:

VeeMAX	example.vee
ATRMax	example.atr
Polarizer	example.pol
RotatIR	example.rot

As an example, the contents of example.vee are shown below:

```
"AutoPRO 5.01"File header
"6 Point Example Profile"        Description
"0"      Not Used
"0"      Not Used
"0"      Not Used
"0"      Not Used
"0"      Not Used
6        Number of points
30,0,#TRUE#,"" Angle, zero, flag, null
40,0,#TRUE#,"" Angle, zero, flag, null
50,0,#TRUE#,"" Angle, zero, flag, null
60,0,#TRUE#,"" Angle, zero, flag, null
70,0,#TRUE#,"" Angle, zero, flag, null
80,0,#TRUE#,"" Angle, zero, flag, null
```

6 Inch Wafer Holder, MappIR. MAP300

These three programmers share the same profile file structure. Each programmer saves the profile with its own extension:

6 inch wafer holder	example.waf
MappIR	example.map
MAP300	example.map

As an example, the contents of example.map are shown below:

```
"AutoPRO 5.01"File Header
"8 Point Example MAP File"      Description
200     Wafer Diameter
5       Edge Exclusion
10      Spot Diameter
“Rectangular” or “Polar”
12632256        Wafer Color
8355711         Spot Color
8       Number of Points in Profile
0,0,#TRUE#,0    Radius, Theta, Flag, zero
55,30,#TRUE#,0Radius, Theta, Flag, zero
55,110,#TRUE#,0         Radius, Theta, Flag, zero
55,145,#TRUE#,0         Radius, Theta, Flag, zero
55,180,#TRUE#,0         Radius, Theta, Flag, zero
55,215,#TRUE#,0         Radius, Theta, Flag, zero
55,250,#TRUE#,0         Radius, Theta, Flag, zero
55,330,#TRUE#,0         Radius, Theta, Flag, zero
```

AutoDiffusIR, X-Y Stage

These two programmers share the same profile file structure. Each programmer saves the profile with its own extension:

AutoDiffusIR	example.apd
XY Stage	example.map

As an example, the contents of example.apd are shown below.

```
"AutoPRO DiffusIR Version 5.00"         File Header
"Description: Sample File"      Description
4       Number of Fields
"Your Company"          Company Name
"Operator"      Field 1 Description
"Part Number"   Field 2 Description
"Size"  Field 3 Description
"Lot Number"    Field 4 Description
        Blank Line
16711680        Operator 1 Color
65280   Operator 2 Color
16776960        Operator 3 Color
255     Operator 4 Color
16711935        Operator 5 Color
65535   Operator 6 Coloer
""      Null

"Joan"  Operator 1
```

"Jim" Operator 2
"Mary" Operator 3
"Bob" Operator 4
"Anne" Operator 5
"Tom" Operator 6
1 Sample Position
"Joan" Operator
"123-456" Field 2 Entry
"Large" Field 3 Entry
"a123" Field 4 Entry
2 Sample Position
"Jim" Operator
"234-5678" Field 2 Entry
"Large" Field 3 Entry
"B234" Field 4 Entry
3 Sample Position
"Mary" Operator
"345-6789" Field 2 Entry
"Medium" Field 3 Entry
"C456" Field 4 Entry
-1 End of sample list

Disk Checker

This program has its own specific format. As an example, the contents of example.lib are shown below:

"AutoPRO 5.0" File header
"Example Lube file" File Description
95 Disk Diameter
3 Inner Edge Exclusion
3 Outer Edge Exclusion
3 Sides to Analyze
4.8 Spot Diameter
1 No. of Radial Positions
4 No. of Angular Positions
30 Radial Position 1
30 Radial Position 2
42 Radial Position 3
32 Radial Position 4
38 Radial Position 5
42 Radial Position 6

Initialization Files

To aid in inter-program communications between AutoPRO and FTIR software packages, a file is generated each time a sample is collected. This file called AP5.ini has the standard structure of a Microsoft Initialization file. If may be written to and read from within Visual Basic using the functions GetPrivateprofilestring and Saveprivateprofilestring.

If you are programming in 16 bit visual basic, the Windows Registry is not available to you. In this case, information on the current spectrum collected is available in this initialization file. An example file is shown below:

```
[IR Setup]          IR Section
Background Scans=4      No. Backgrnd scans
Sample Scans=4No. Sample Scans
High Wavenumber=4000            High Wavenumber
Low Wavenumber=400  Low Wavenumber
Resolution=4      Resolution
Spectrum Format=Transmission Spectral Format
Macro Directory=C:\Program Files\AutoPRO7\Macro      Macro Directory
Spectra Directory=C:\AUTOPRO7\Spectra            Spectra Directory
Profile Directory=C:\VB5\apshim            Profile Directory
IR Path=C:\Program Files\Bio-Rad\FTIR Software\Bin\     IR Software Path
Background Name=C:\AUTOPRO\Spectra\Back   Background name
Sample Name=C:\AUTOPRO\Spectra\9968232    Sample Name
AutoPRO Top=8280        Window Position
AutoPRO Width=11505  Window Position

[Point]   Point Section
Entries=6           No. of Valid Entries
Number=5          No. Points in profile
Point=5             Current Point
Line1=Six Inch    Accy Description
line2=66          Radius Value
line3=360         Angle value
line4=Size =      Not valid > 6
line5=Sort Code =           Not valid > 6
line6=Description =       Not valid > 6
line7=Stuff =     Not valid > 6

[Peak Reporter] My Program Section
Peak Threshold=1.23
Start Wavenumber=4000
End Wavenumber=400
```

Registry

NOTE: Changing your registry settings can have disastrous consequences. PIKE recommends that you do not change any setting in the registry – Ever. You may, however read any of the registry settings from within a Visual Basic program (Version 5 or 6) by using the getsetting function in Visual Basic. The information below is for reference only.

All the setup files and settings for AutoPRO are saved in the Windows registry. To help in accessing the registry settings, the location of these settings is the default location as defined by the Microsoft visual Basic getsetting function. To view registry settings, perform the following:

1. Click on Start and select run
2. Type into the text box REGEDIT
3. The registry editor will open
4. Select HKEY_CURRENT_USER
5. Select Software
6. Select VB and VBA Program Settings
7. Select AutoPRO

There are several folders in the AutoPRO Section:

MAIN	AutoPRO Control Settings Settings
APV	VeeMax, ATRMax, Polarize, RotatIR Settings
APW	6" wafer, MappIR, MAP300 Settings
APD	AutoDiffusIR Settings
APL	Disk Lubrication Settings
APXY	AutoXY Settings
APA	6" Autosamp, 8" AutoSamp, 12" AutoSamp Settings
APVP	VeeMax/ Polarizer, ATRMax.Polarizer Settings
SYSTEM	AutoPRO System Settings
DATA COLLECT	Saves info on each sample after data collection
RESULTS	Used by the APRES program to store values
IR SETUP	Used to save IR Data Collection parameters

Below is a list of registry settings with a brief description of each:

[HKEY_CURRENT_USER\Software\VB and VBA Program Settings\AutoPRO\Main]

"BaudRate"="9600"	Baud Rate
"CommPort"="1"	Communications Port
"Random"="False"	Diagnostic, sets up infinite random motion.
"Diagnostic"="0"	Diagnostic Setting, shows diagnostics
"Demo"="True"	Accessory Demo Mode Flag
"Type"="21"	Accessory Type VeeMax=1 ATRMax=2

Polarizer=3
RotatIR=4
6" Wafer Holder=11
8" Wafer Holder=12
MappIR=13
AutoDiffusIR=15
Map300=16
Lubrication Checker=17
XY Stage=18
VeeMax/Polarizer=21
ATRMax/Polarizer=22

"IRDemo"="False" IR Bench Coupled Flag
"Background"="4" Number of Background Scans
"Sample"="4" Number of Sample Scans
"Highwn"="4000" High Wavenumber Limit
"Lowwn"="400" Low Wavenumber Limit
"Resolution"="4" Resolution
"Format"="Absorbance" Spectrum Format
Absorbance
Transmission
Single Beam
Interferogram
"IRPath"="C:\\WIN-IR\\" IR Software Path
"IRName"="Win-ir.exe" IR Software Name
"IRBench"="Bio-Rad Win-IR" IR Bench Description
"First1"="8" Motor 1 Initial Rate
"First2"="10" Motor 2 Initial Rate
"Slope1"="15" Motor 1 Accel Slope
"Slope2"="15" Motor 2 Accel Slope
"Last1"="12" Motor 1 Final Rate
"Last2"="15" Motor2 Final Rate
"Microstep1"="2" Motor 1 Microstepping
"Microstep2"="2" Motor 2 Microstepping
"MicroFlag"="True" MicroStepping Flag
"PathFilename"=""
"Macro"="" Macro Default Directory
"Spectra"="" Spectra Default Directory
"Profile"="C:\AutoPRO5\Profile" Profile Default Directory
"Pre Experiment Macro File"="C:\fileinfo.ab" Pre Exp Macro Path/Name
"Post Experiment Macro File"="C:\Mfutils.ab" Post Exp Macro Path/Name
"Pre Sample Macro File"="C:\Function.ab" Pre Samp Macro Path/Name
"Post Sample Macro File"="C:\Quantbas.ab" Post Samp Macro Path/Name
"Spectra Extension"=".spc" Spectral File Extension
"Macro Extension"="AB" Macro File Extension
"Macro Filter"="Array Basic File (*.AB)|*.Bas|All Files (*.*)|*.*|" Filter
"IR File Extension"="spc"
"Background All"="True" Background All Flag
"Filename Type"="3" Filename Type

```
                                                    Generate=1
                                                    8 Char Numeric=2
                                                    Base Name=3
"Filename Base"="AP"                                BaseName
"Selfile"="0"                                       Filename Builder Select
"Startfile"="11111"                                 Filename Builder Start
"Lenfile"="11111"                                   Filename Builder length
"Orderfile"="12345"                                 Filename Builder Order
"Recent10"="C:\AutoPRO5\Profile\example.VEE"        Recent VeeMax File
"Recent11"=""                                       Recent VeeMax File
"Recent12"=""                                       Recent VeeMax File
"Recent13"=""                                       Recent VeeMax File
"Recent20"="C:\AutoPRO5\Profile\Example.ATR"        Recent ATRMax File
"Recent21"=""                                       Recent ATRMax File
"Recent22"=""                                       Recent ATRMax File
"Recent23"=""                                       Recent ATRMax File
"Lock1"="255"                                       Lock Code
"Lock2"="7"                                         Lock Code
"Recent30"="C:\AutoPRO5\Profile\Example.pol"        Recent Polarizer File
"Recent31"=""                                       Recent Polarizer File
"Recent32"=""                                       Recent Polarizer File
"Recent33"=""                                       Recent Polarizer File
"Recent40"="C:\AutoPRO5\Profile\Example.ROT"        Recent Polarizer File
"Recent41"=""                                       Recent RotatIR File
"Recent42"=""                                       Recent RotatIR File
"Recent43"=""                                       Recent RotatIR File
"Recent110"="C:\AutoPRO5\Profile\Example.WAF"       Recent Wafer File
"Recent111"=""                                      Recent Wafer File
"Recent112"=""                                      Recent Wafer File
"Recent113"=""                                      Recent Wafer File
"Recent130"="C:\AutoPRO5\Profile\Example.MAP" Recent MappIR File
"Recent131"=""                                      Recent MappIR File
"Recent132"=""                                      Recent MappIR File
"Recent133"=""                                      Recent MappIR File
"Recent150"="C:\AUTOPRO\3.apd"                      Recent AutoDiffusIR File
"Recent151"=""                                      Recent AutoDiffusIR File
"Recent152"=""                                      Recent AutoDiffusIR File
"Recent153"=""                                      Recent AutoDiffusIR File
"Recent170"="C:\AutoPRO5\Profile\Example.LUB"       Recent Lube File
"Recent171"=""                                      Recent Lube File
"Recent172"=""                                      Recent Lube File
"Recent173"=""                                      Recent Lube File
"Recent180"="C:\AutoPRO5\Profile\Example.XYA" Recent AutoXY File
"Recent181"=""                                      Recent AutoXY File
"Recent182"=""                                      Recent AutoXY File
"Recent183"=""                                      Recent AutoXY File
"Recent210"="C:\AUTOPRO\3.vep"                      Recent VeeMax/Polr File
"Recent211"=""                                      Recent VeeMax/Polr File
```

"Recent212"="" Recent VeeMax/Polr File
"Recent213"="" Recent VeeMax/Polarizer File
"Recent220"="C:\AutoPRO5\Profile\3.atp" Recent ATRMax/Polr File
"Recent221"="" Recent ATRMax/Polr File
"Recent222"="" Recent ATRMax/Polr File
"Recent223"="" Recent ATRMax/Polr File

[HKEY_CURRENT_USER\Software\VB and VBA Program Settings\AutoPRO\APV]
"Height"="4000" Window Location
"Width"="5300" Window Location
"Left"="9015" Window Location
"Top"="3015" Window Location

[HKEY_CURRENT_USER\Software\VB and VBA Program Settings\AutoPRO\APVP]
"Height"="4600" Window Location
"Width"="6000" Window Location
"Left"="4680" Window Location
"Top"="3460" Window Location

[HKEY_CURRENT_USER\Software\VB and VBA Program Settings\AutoPRO\APW]
"Diameter"="200" Wafer Diameter
"Beam"="8" Beam Diameter
"Edge"="5" Edge Exclusion
"R Offset"="0" Radius Offset
"T Offset"="0" Theta Offset
"units"="mms" Units
"Height"="4600" Window Location
"Width"="6000" Window Location
"Left"="4680" Window Location
"Top"="3460" Window Location

[HKEY_CURRENT_USER\Software\VB and VBA Program Settings\AutoPRO\APD]
"Height"="5325" Window Location
"Width"="6000" Window Location
"Company"="PIKE" Company
"NumField"="5" Number of Description Fields
"Field 0"="Operator" Field Name
"Field 1"="description2" Field Name
"Field 2"="description3" Field Name
"Field 3"="description4" Field Name
"Field 4"="description5" Field Name
"Operator 1"="" Operator Name
"Operator 2"="" Operator Name
"Operator 3"="" Operator Name
"Operator 4"="" Operator Name
"Operator 5"="" Operator Name
"Operator 6"="" Operator Name
"Colors"="yes" Assign Colors to Operator

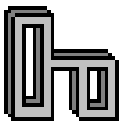
[HKEY_CURRENT_USER\Software\VB and VBA Program Settings\AutoPRO\APL]

"Top"="3712"	Window Location
"Left"="4747"	Window Location
"Diameter"="95"	Disk Diameter
"Beam"="6.4"	Beam Diameter
"InnerEdge"="5.00"	Inner Edge Exclusion
"Outeredge"="5.00"	Outer Edge Exclusion
"Radius 1"="21.00"	Radius 1 Value
"Radius 2"="0.00"	Radius 2 Value
"Radius 3"="0.00"	Radius 3 Value
"Radius 4"="0.00"	Radius 4 Value
"Radius 5"="0.00"	Radius 5 Value
"Radius 6"="0.00"	Radius 6 Value
"NumRadius"="1"	Number of radius loactions
"NumAngle"="4"	Number of angle locations

[HKEY_CURRENT_USER\Software\VB and VBA Program Settings\AutoPRO\APXY]

"Height"="4600"	Window Location
"Width"="6000"	Window Location
"Company"="PIKE"	Company Name
"NumField"="5"	Number of Description Fields
"Field 0"="Key"	Field Name
"Field 1"="description2"	Field Name
"Field 2"="description3"	Field Name
"Field 3"="description4"	Field Name
"Field 4"="description5"	Field Name
"Operator 1"=""	Operator Name
"Operator 2"=""	Operator Name
"Operator 3"=""	Operator Name
"Operator 4"=""	Operator Name
"Operator 5"=""	Operator Name
"Operator 6"=""	Operator Name
"Well Size"="96"	Well Size
"Colors"="yes"	Assign Colors to Operator
"Left"="4680"	Window Location
"Top"="3460"	Window Location

Appendix A



Nicolet OMNIC Example

The Nicolet MACROS\BASIC program is a convenient way in which to build macros to perform automated experiments. Since MACROS\BASIC does not have the facility for passing command line arguments in a call to an external (EXE) program, the following six programs have been provided in order to program your accessory from within MACROS\BASIC:

1. **INIT.EXE**
   Initialize accessory. AutoPRO communicates with and sets up the Motor Controller. The accessory is then initialized to the home position.

2. **NEWFILE.EXE**
   When this command is performed, the file dialog box is opened and a file containing the coordinates to be measured may be selected.

3. **NEXT.EXE**
   Move to the next point in a profile. If the end of the profile has been reached, nothing happens.

4. **FIRST.EXE**
   This program moves the accessory to the first point in the profile.

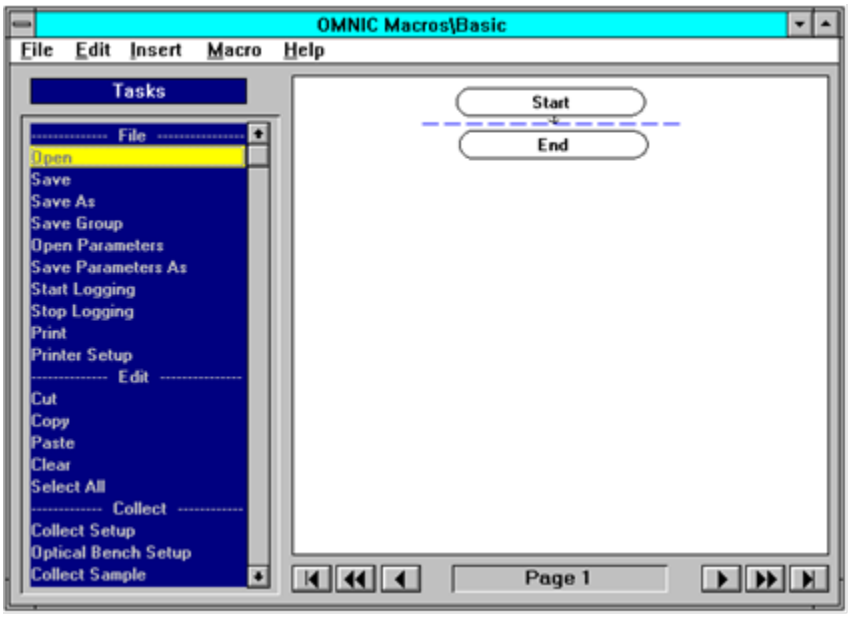
5. **UNLOAD.EXE**
   This program unloads the accessory. The next command must be LOAD.EXE

6. **LOAD.EXE**
   This program loads the accessory. The accessory is moved to its home position.

We will step through the creation of a simple macro to illustrate the use of the program MOTOR.EXE within a macro.

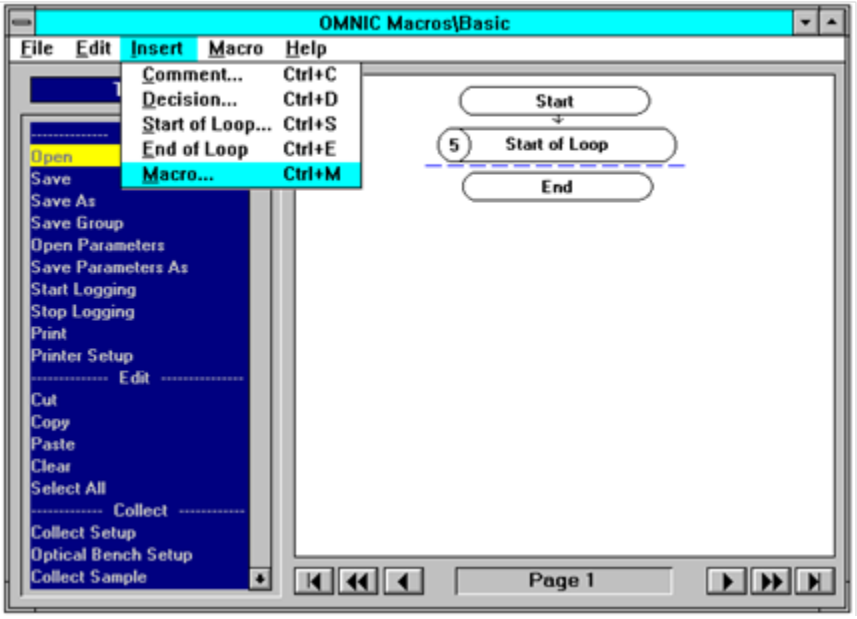
OMNIC Macro

1. Open OMNIC Macros\Basic by clicking on the Macros\Basic icon in the OMNIC program group. The display shown below will appear.

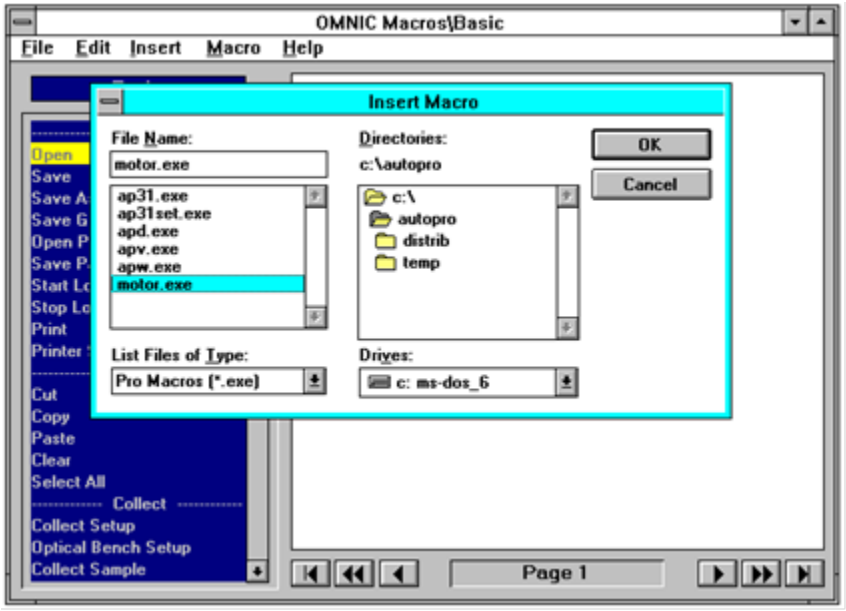


2. In order to perform repeated motions with AutoPRO, a program loop must be constructed. From the INSERT Menu, click on START OF LOOP. A dialog box will appear, requesting the number of loops to perform. Enter a number which is equal to the number of points in the profile that you wish to run.

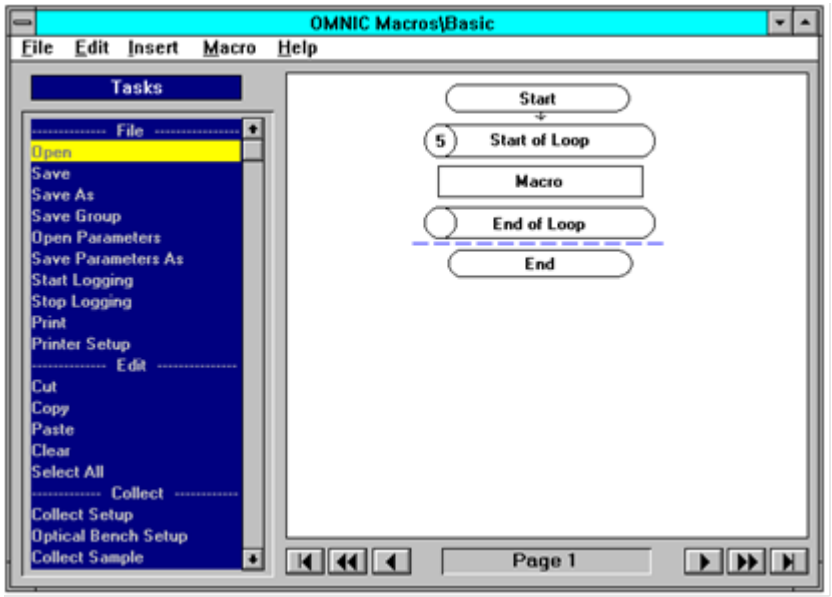
3. From the INSERT Menu, click on MACRO. A file dialog box will appear.



4. Insert the NEXT.EXE program:
In the List Files of Type: box, select Pro Macros (*.exe).
Select C:\Autopro from the Directories box.
Finally in the FileName Box, select NEXT.EXE.
Click on OK. The AutoPRO motor program, NEXT.EXE will be inserted into the macro.



Close the end of loop by selecting the INSERT menu and clicking on End of Loop.



The first time that the program NEXT.EXE is run, the AutoPRO window is opened and the command NEXT is sent to AutoPRO. If a profile file has not already been selected, AutoPRO will open the File dialog to allow you to select a file. The accessory is then initialized and moved to the first point in the profile. On subsequent calls to NEXT.EXE, the accessory is moved to the next point. If the last point has been reached, nothing happens.

A simple macro has been constructed to move the automated accessory to different positions. You may test the function of the macro by selecting the MACRO menu and clicking on Test.

Save the macro by selecting Save from the File menu.

This macro may be assigned a button in the OMNIC Macro Panel Program. Consult your OMNIC Macro Panel documentation for instructions on how to do this.

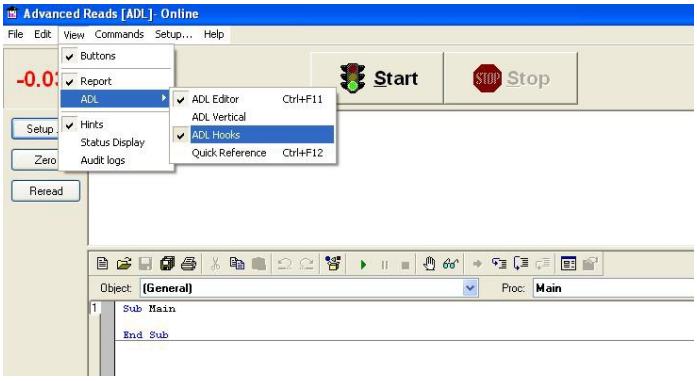
AutoPRO for Cary Win UV

Introduction

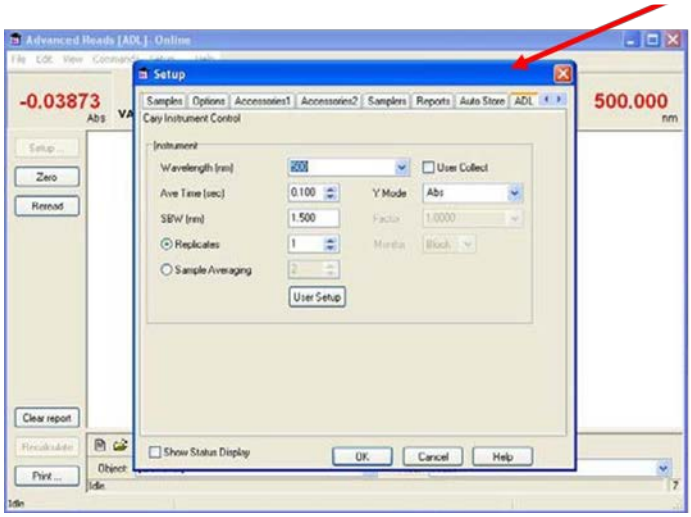
This is an addendum to the AutoPRO manual. Its purpose is to explain how to use AutoPRO software for operation with the Cary Win UV series spectrometer.

AutoPRO can host or be a client during an experiment run. The experiment run includes configuring the spectrometer for data collection, instructing the PIKE stage when to move, collecting data, data workup and data storage. In the case of the Cary series spectrometers AutoPRO acts like a client. When the Advanced Reads or Scan application is run and the ADL hooks option is enabled, AutoPRO will only move the stage when instructed. All the collection parameters that are set in the Cary/Setup window will be used.

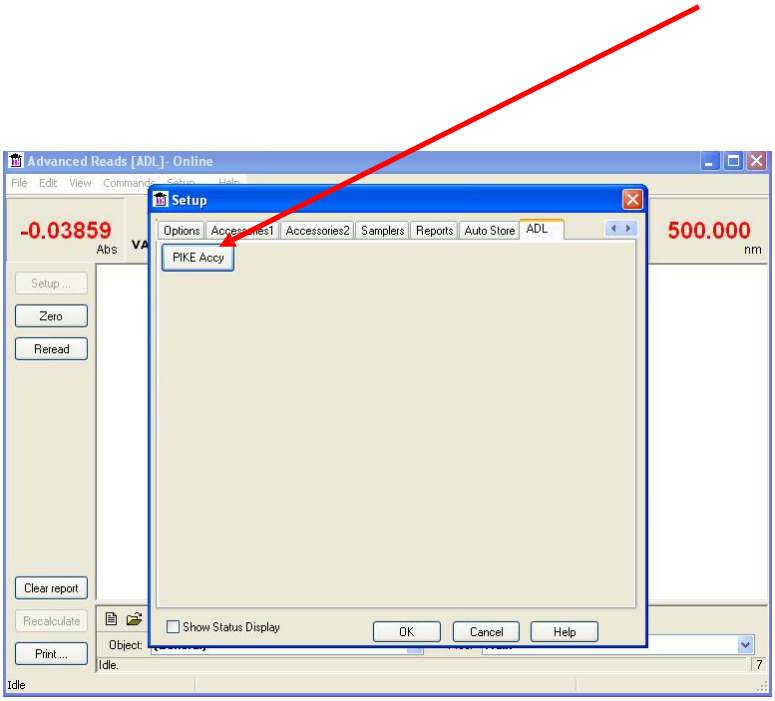
After installing the AutoPRO5 software the ADL hooks option must be set in the Cary software application, either via Advanced Reads or Scan. Proceed to the start menu and select the Advanced Reads/Scan application:



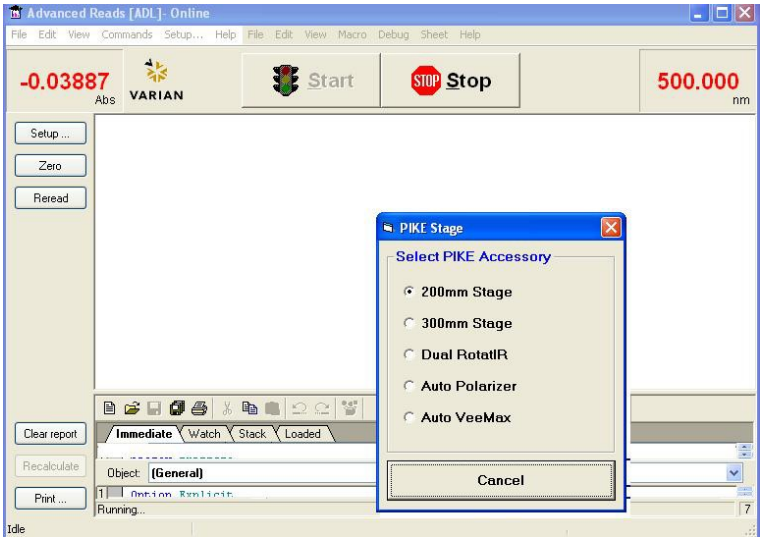
Select View/ADL/ADL hooks and ensure there is a check mark for this option. This will produce a new tab in the setup window. You may have to scroll to see the new tab.



Clicking on this ADL tab will bring up the following menu. You will see a new button added:

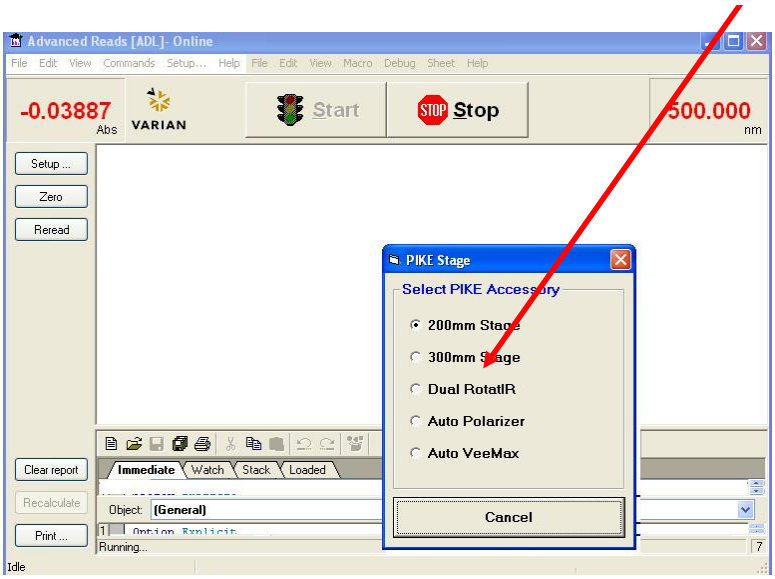


Clicking on this button will bring up the main accessory selection menu. This menu allows the user to select from different accessories. Depending on the accessory being used different dialog boxes will appear.



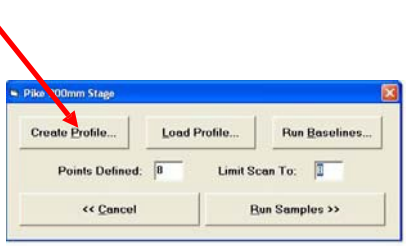
Collecting Data with Your PIKE Accessory

NOTE: Prior to performing the following, please ensure all data collection parameters are set in the setup window. From the main access

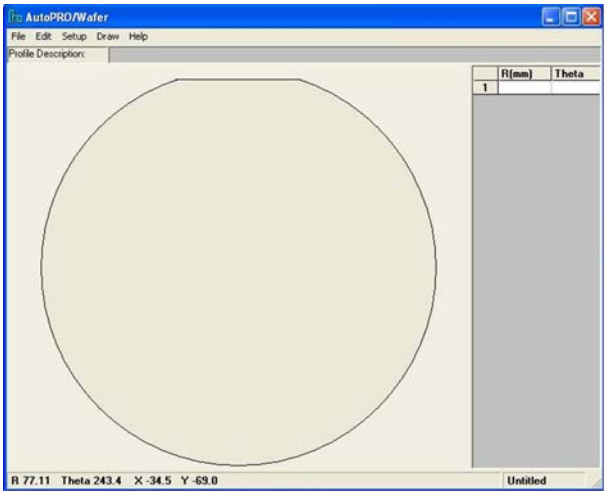


This will open the following window:

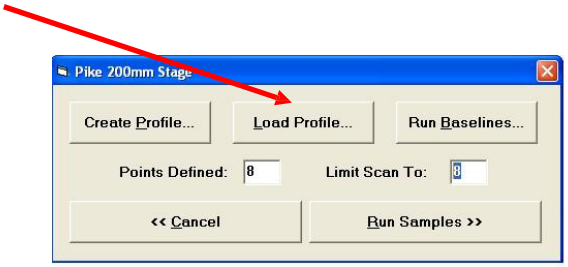
Clicking on the Create Profile button will allow the user to create a file that contains the desired locations to collect data. This is called a “profile” file.



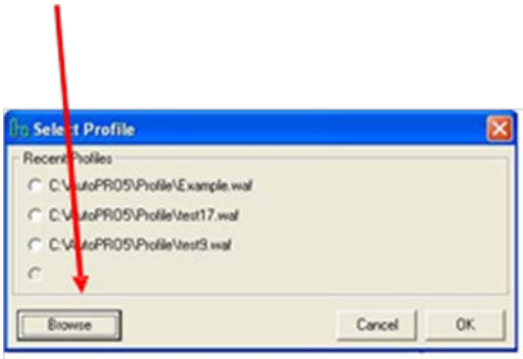
The following window will open up allowing the user to program positions in one of three ways, load a predefined map, enter positions in the grid or point and click. For loading a predefined map select Draw from the main menu. From here you can select from three different predefined profiles or program new ones using polar or Cartesian coordinate systems. To enter positions in the data grid on the right hand side of the display, simply click on the first cell under the R (mm) column and enter the radial value for the position. Hit Enter then enter the Theta value.



For point and click, hover the mouse over the wafer surface and click on the points for sampling. This can be associated with a grid that is set under the Draw menu. When finished, select File/Save…Then close the window. After a profile has been created and saved, you can then load it by selecting the Load Profile button.

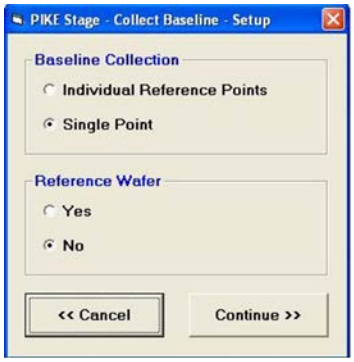


This allows the user to navigate to any profile that has been created using the most recent profiles to start or via browsing.



Once a profile has been loaded data collection can commence. Either a baseline or multiple baselines can be run or sample spectra can be collected.

When the Run Baselines button is selected the following will appear.



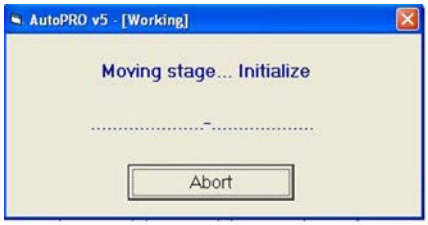
The user has the following options: Collect a single baseline with or without a reference wafer, or collect multiple baselines at each point in the profile with or without a reference wafer.

After selecting which baseline option to use, the following window will appear. This is where you define the spectral filename, type (individual spectra or a single multifile) and location of where to save it. If you want to change the name, click on the ellipse:

If a reference wafer is going to be used, click on Continue the stage will subsequently initialize and unload allowing the user to load a reference wafer.

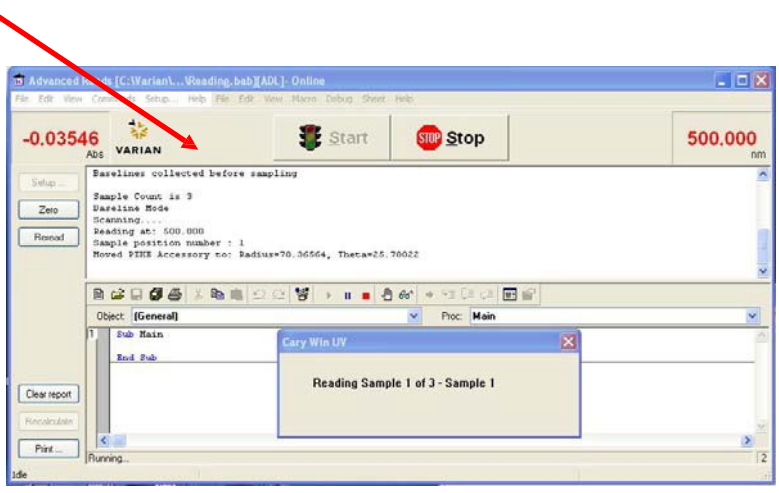
Once unloaded, the following prompt will appear.

Click on OK when the reference wafer is loaded and the stage will move in.

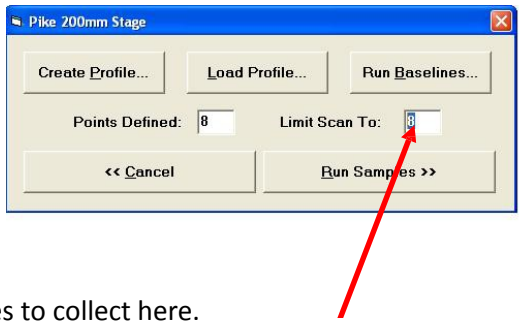


Once the stage has reinitialized it will then proceed to the first point of the profile.

And start the data collection. The results will be saved in the data base and displayed in the report.



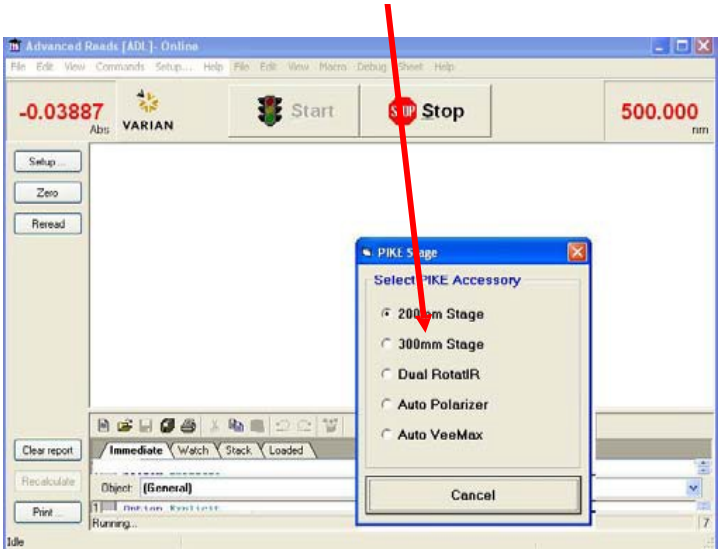
After all the baselines are collected the stage will unload if a reference wafer is being used, prompt the user to load the sample and then the following window will reappear:



Select the number of samples to collect here.

Click on Run Samples to move the stage to the same sample positions as the reference and subsequently collect/save the sample data.

Once back in the main menu, click on the accessory name again to repeat.



Replacement Parts and Options

The following parts and options may be ordered for AutoPRO Software.

Part Number	Description
007-040000	AutoPRO Software V5