SPECTRUM

User's Guide

PerkinElmer®

Setup and Administration

Setup and Administration

These topics describe the range of Setup and Administration commands that enable you to:

Administer the login names and passwords (if required) for each Spectrum user. To set up users, you must be logged into Spectrum as an Administrator.

Administer the list of instruments available to Spectrum.

Set up the connected Instrument.

Set up instrument Ready Checks.

Set up Instrument Verification.

Setup the connected Raman Instrument.

Verify and calibrate the connected Raman Instrument.

Set up the custom Export of your spectra.

Set up the email account that will be used for Send To Email.

Set up how peaks in your spectra are detected and labeled.

Setup the default graph View.

Set up the Compare function.

Set up the Biodiesel process (available if you have the Biodiesel Analyzer installed).

Set up Spectral Libraries and Search Parameters.

Setup the MultiSearch function (available if you have a MultiSearch license).

Setup the Adulterant Screen function (available if you have an Adulterant Screen license).

Set up the Verify function.

Set up the Quant process.

Define, or edit, a Macro that applies a series of process commands to your spectra.

Define, or edit, an Equation to perform calculations on one or more spectra, or on the data obtained from other processes.

Administration

Provided that you are logged into Spectrum Standard or Spectrum ES as an administrator, the Administration sub menu of the Setup menu enables you to:

- Setup a login name and password (if required) for each Spectrum user.

Provided that you are logged into Spectrum ES as an administrator, the Administration sub-menu of the Setup menu also enables you to:

- Add new Groups and set the permissions for each group (except Administrators).
- Define the operations in the software that require a Signature from a pre-defined list.
- Administer the Users Audit Trail.
- Set a default workspace for a group

Setting up Users, Groups and Passwords

Each person using Spectrum must be set up as a user by a person who has permission to perform administration tasks.

- To set up users, select **Administration** from the Setup menu, and then click **Setup Users.**

  The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.

NOTE: When making any changes in the dialog, click **Apply** to accept the changes and keep the dialog open. Click **OK** to apply the changes and close the dialog.

A user's access rights depend entirely on group memberships. Spectrum Standard utilizes two pre-defined groups, namely the Administrators group and the Users group. You cannot use Spectrum to amend the access rights applied to these groups or to create new groups. The default Spectrum user named Administrator has membership of both the Administrators group and the Users group for Spectrum standard.

In Spectrum Enhanced Security (ES), the Administrators, Users, Reviewers and Approvers groups are predefined. The access rights applied to the Users, Reviewers and Approvers groups can be customized, and additional groups with particular access rights created. The access rights applied to the Administrators group cannot be customized.

The Administrators group exists for a range of PerkinElmer software applications. The Users group exists for the standard versions of a range of PerkinElmer software and for Spectrum ES (version 10.3 or later), but not for other ES versions of PerkinElmer software, including Spectrum version 6 ES.

A user defined for another standard PerkinElmer application (including Spectrum version 6) will appear in the Users list for Spectrum, but that user must be enabled by a Spectrum administrator.

Additional Information

Managing Users

- Default Users
- Adding a New User
- Assigning a User to a Group; Removing a User from a Group
- Enabling or Disabling a User; Deleting a User

Managing Groups

- Default Groups
- Adding a New Group
- Deleting a group
- Defining the Permissions for a Group

Signatures

- Defining the Settings for a Signature Point

Default Users

The following user is pre-defined for Spectrum:

User	Password	Group Membership
Administrator	administrator	Administrators, Users

The following user is pre-defined for Spectrum ES:

User	Password	Group Membership
Administrator	administrator	Administrators

Additional Information

Default Groups

Assigning Users to and Removing Users from a Group

Default Groups

Spectrum Standard

The following groups are predefined for Spectrum. These groups cannot be deleted or other groups added.

Group	
Users	Members of the Users group cannot set up other users.
Administrators	Only members of the Administrators group have access to the Setup Users command.

Spectrum ES

The following groups are predefined for Spectrum ES. The Administrators group cannot be deleted. Other groups can be deleted or other groups added.

Group	
Administrators	Only members of the Administrators group have access to the Setup Users command. The permissions for the Administrators group cannot be changed.
Users	By default, members of the Users group can perform all functions in the software except those associated with Administrators, and Return Workspace, Review and Approve. The permissions available are defined by the Administrator. Members of the Users group cannot set up other users.
Reviewers	Members of the Reviewers group are intended to act as reviewers of changes made by other users requiring an electronic signature. Members of the Reviewers group cannot set up other users.
Approvers	Members of the Approvers group are intended to act as approvers of changes made by other users requiring an electronic signature. Members of the Approvers group cannot set up other users.

Additional Information

The Administrators group applies across a range of PerkinElmer software applications.

Both the Administrators and Users groups are utilized by Spectrum version 6, so a user defined for Spectrum version 6 is also valid for Spectrum version 10. For Spectrum version 6, the password for the default Administrator expires after 42 days.

The Users group does not exist in some other ES (Enhanced Security) versions of PerkinElmer software applications, including Spectrum version 6 ES.

Adding a New User to Spectrum

Use the Setup Users command to add a user to the list of users that are able to log in to Spectrum at this PC.

You cannot add a user unless you are logged into Spectrum as an administrator.

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.

2. Select the Password Control tab.

   If the **Login Type** is **Windows**, which is a global setting, click **Cancel**.

   Add new users using Windows User Management.

   Otherwise:

3. Select the Users tab and click **New**.

   The New User dialog is displayed.

4. Enter the **User name** and **Full name**.

5. If the **Login Type** is **PerkinElmer Login**, enter a user **Password**, and then enter this password again in the **Confirm password** field.

   The global properties of passwords, such as their minimum length, are defined on the Password Control tab. Passwords are case-sensitive, and can consist of letters, numbers and single spaces only.

6. By default, the **Status** of the user is **Enabled**, which allows the user to log in straightaway. If you want to enable the login later, select **Disabled**.

   When you enable a previously disabled user, you must enter a new password and confirm it.

7. If the **Login Type** is **PerkinElmer Login**, select whether the User must change their password at the next login.

   NOTE: In Spectrum ES **User must change password at next login is mandatory.**

8. Click **OK**.

   The User name drop-down list is updated with the new user.

Adding and Deleting a Group (Spectrum Enhanced Security Only)

Use the Setup Users command to add a new group to those that users can be assigned to in Spectrum Enhanced Security at this PC.

NOTE: It is not possible to create a new group within the Standard version of Spectrum.

You cannot add a group unless you are logged into Spectrum as an administrator.

Administrators can assign permissions to the members of a group that control what they are able to do in a way that is tailored to your company's working practices. For example, you can set up permissions that allow members of a particular group to run a Compare process, but not to modify the Compare parameters, such as the Correlation value, or the spectra that are used as the Compare references.

If a group does not have permission to edit a group of options, those options will not be visible in the software. For example, if you do not have permission to run a Deconvolution Process, that option will not be displayed on the Process menu. If you do not have permission to perform any of the processes on the Process menu, then the menu will be hidden.

Adding a New Group

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users, Groups, Signatures and Passwords Control dialog is displayed.
2. Select the Groups tab and click **New**.

   The New Group dialog is displayed.
3. Enter the **Group name**.
4. Click **OK**.

   The new group is created.
5. Click **OK** to close the dialog, or select the Permissions and available Instruments for the group.

Deleting a Group

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users, Groups, Signatures and Passwords Control dialog is displayed.
2. Select the Groups tab.
3. Select the **Name** of the Group you want to delete from the drop-down list.
4. Click **Delete**.

   A confirmation dialog asks if you are sure that you want to delete the group.

5. Click **Yes**.

   The group is deleted.

NOTE: Users that are not a member of a group are not able to access Spectrum. If you delete a group that has users assigned to it, check that all users are members of another group.

Defining What Members of a Group Can Do

To define with what members of a group are able to do:

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users, Groups, Signatures and Passwords Control dialog is displayed.

2. Select the Groups tab.
3. Select the **Name** of the Group you want to modify from the drop-down list.
4. Click **Show Permissions** if the permissions are not displayed.

   The Permissions area shows the available permissions for the group.

   A tick indicates that the permission is selected for the group.

5. Select or deselect the **Permissions** for the members of the group.

   To select all the available permissions, select the **Permissions** option at the top of the list.

   The following table lists the default permissions for the pre-defined groups in Spectrum:

Group	Default permissions
Administrators	The permissions of this group cannot be edited, and are not listed. Only members of the Administrators group are able to perform Administration tasks – setup users, groups and passwords.
Users	All tasks are enabled except Return Workspace, Review and Approve.
Reviewers	Review, Return Workspace, Import Sample Table Setups, Export Sample Table Setups, Import IR Instrument Setup, Export IR Instrument Setup, Setup Macros and Setup Equations only.
Approvers	Approve, Return Workspace, Import Sample Table Setups, Export Sample Table Setups, Import IR Instrument Setup, Export IR Instrument Setup, Setup Macros and Setup Equations only.

6. Select **Show Instruments**.

7. Select the instrument or instruments that you want the members of the group to be able to use.

   To select all the available instruments, check the **Instruments** option at the top of the list.

NOTE: When a new instrument is added to the Spectrum software, it will automatically be added to the instruments available for every group.

8. Click **Apply** to apply the settings to the group and keep the dialog open, or **OK** to apply the settings and close the dialog.

Additional Information

An Administrator can define a default workspace (software settings, workspace layouts and objects such as equations, macros, sample table setups, and instrument setups) for each group.

Assigning Users to, and Removing Users from, a Group

If you are an administrator, you can assign a Spectrum Standard user to the Administrators group, the Users group, or both. You can assign a Spectrum Enhanced Security user to the default groups Administrators, Users, Approvers and Reviewers, or to any new groups created by an administrator.

To Assign a User to a Group

1. From the Setup menu, select **Administration** and then click **Setup Users.**

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.
2. Select the Users tab, and then the user's **Name** from the drop-down list.
3. Select the Group from the list of **Available groups for user** and then click **Add.**

   The Group is added to the **User is a member of list**, and removed from the **Available groups for user list.**

To Remove a User from a Group

1. From the Setup menu, select **Administration** and then click **Setup Users.**

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.
2. Select the User tab, then the user's **Name** from the drop-down list.
3. Select the Group from the list of **Available groups for user** and then click **Remove.**

   The Group is removed from the **User is a member of list**, and added to the **Available groups for user list.**

Additional Information

Disabling, or Deleting, a User

Adding and Deleting a Group

Enabling, Disabling or Deleting a User

NOTE: These procedures are not applicable when Login Type is set as Windows Login on the Password Control tab of the Users and Password Control dialog. In this case, add or delete users using Windows User Management.

To Disable an Existing User

1. From the Setup menu, select **Administration** and then click **Setup Users .**

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.

2. Select the Users tab, select the user's **Name** from the drop-down list, and then click **Edit.**

   The Edit User dialog is displayed.

3. In the Status area, select **Disabled**, and then click **OK.**

   When this user attempts to login the error message 'Your user name has been locked or disabled. Please contact your system administrator' will be displayed.

NOTE: To enable a previously disabled user, select **Enabled** on this dialog, and then enter a new Password and confirm it. The **User must change password at next login** selection is recommended.

To Delete a User

1. From the Setup menu, select **Administration** and then click **Setup Users.**

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.

2. Select the Users tab, select the user's **Name** from the drop-down list, and then click **Delete.**

   A User Administration message will be displayed asking you to confirm that you wish to delete the user.

3. Click **Yes.**

   The user is deleted.

NOTE: It is not possible to re-use a User name that has been deleted.

NOTE: It is not possible to delete the Administrator.

Signatures (Spectrum Enhanced Security Only)

Signatures are only available in Spectrum ES. An electronic signature as defined by 21 CFR Part 11 means a computer data compilation of any symbol or series of symbols executed, adopted, or authorized by an individual to be the legally binding equivalent of the individual's handwritten signature.

In Spectrum ES software, all operations that cause data to be collected, administer security or cause spectra and results data to be saved have an associated Signature Point that requires a signature. The list of Signature Points within the software is pre-defined, and includes:

- Loading and saving instrument settings files.
- Reporting on ready checks and instrument validation.
- Generating reports.
- Exporting data.
- Deleting graphs.
- Creating or making changes to equations and macros.
- Approving and reviewing items that have been signed by other users.

When a Signature Point occurs in the software, a dialog will appear prompting you to enter your User name and Password, and then select a pre-defined Reason from the drop-down list, if required. In the Comments section you can add any additional information.

Members of the Administrators group are able to define whether a signature and comment is required for each Signature Point individually, or apply the same settings to all Signature Points. In addition, for each Signature Point they can define the list of Reasons.

NOTE: If **Signature required** is not selected for a signature point, you will not be prompted for a signature. However, if any Reasons have been set up for the signature point, you will still be prompted to select one.

Defining the Settings for a Signature Point

1. From the Setup menu, select **Administration** and then click **Setup Users**. The Users, Groups, Signatures and Passwords Control dialog is displayed.
2. Select the Signatures tab.

3. Select the Signature Point **Name** from the drop-down list of available signature points.

   The following signature points are available in Spectrum:

Signature Point	**Description**
Approve	Occurs on demand. See Reviewing and Approving for more information.
Data	Occurs when data is added to the database, for example, when opening a spectrum that was collected on another system.
Data Export Collection	Occurs when data is exported immediately after data collection. See Setup Instrument - Data Collection.
Delete Graph	Occurs when a user deletes a spectrum or Samples View from the Data Explorer. The spectra are added to the Recycle Bin.
Equation	Occurs on demand, accessed via the Setup Equations tab. If you attempt to export an unsigned equation, you will be prompted for a signature first. If you import an equation, you will be prompted for a signature first. If you exit Spectrum and have unsigned Equations, the Equation will be signed for when you sign the workspace.
Instrument Validation	Occurs immediately after selecting to run a Instrument Validation.
IR Instrument Setup	Occurs on demand, accessed via the Instrument Settings dialog, or when you exit Spectrum software. If you attempt to export an unsigned instrument setup, you will be prompted for a signature first. If you import an instrument setup, you will be prompted for a signature first. See Load and Save for more information.
Macro	Occurs on demand, accessed via the Setup Macros tab. If you attempt to export an unsigned macro, you will be prompted

	for a signature first. If you import a macro, you will be prompted for a signature first. If you exit Spectrum and have unsigned macros, the macro will be signed for when you sign the workspace.
Output	Signature is demanded just before the output of data. This is before saving, printing or exporting data, and includes saving a report using the **Report** command on the File menu, and saving a report as part of an Output step in a Macro.
Raman Instrument Setup	Occurs on demand, accessed via the Instrument Settings dialog, or when you exit Spectrum software. If you attempt to export an unsigned instrument setup, you will be prompted for a signature first. If you import an instrument setup, you will be prompted for a signature first. See Load and Save for more information.
Ready Check	Occurs immediately after selecting to run a Ready Check.
Review	Occurs on demand. See Reviewing and Approving for more information.
Sample Table Setup	Occurs on demand, or when you exit Spectrum software. If you attempt to export an unsigned sample table setup, you will be prompted for a signature first. If you import a sample table setup, you will be prompted for a signature first. See Sample Table Setups for more information.
Workspace	Occurs on demand, or when you exit Spectrum software. The signature applies to the whole workspace, and covers all currently unsigned activities logged for the user. See Signing for more information.

4. If a Signature is required for a Signature Point, select **Signature required**.
5. If you wish the user to be able to add comments, if required, select **Prompt for comments**.

   When the Signature Point dialog is displayed in the software, the user will be prompted to select a reason. The list of reasons is also defined on this tab.

6. To add a new reason, click **New** and enter the new Reason in the New Reason dialog.

   The reason is added to the list of reasons for the Signature Point.

   OR

   To delete a reason, select the Reason from the Reasons list and click **Delete**.

   You will be asked to confirm that you want to delete the reason. Click **Yes**.

   The Reason is deleted from the **Text** field. The changes are recorded in the Audit Trail.

   OR

   To edit a reason, select the Reason from the Reasons list, click **Edit** and modify the text in the Edit Reason dialog.

   The Edit Reason dialog closes and the updated reason appears in the **Text** field. The changes are recorded in the Audit Trail.

7. Repeat as many times as necessary to add reasons for the Signature Point.
8. When you have finished adding reasons for the Signature Point, reorder the reasons, if required.

   Items will appear in the Reason drop-down list in the order they are listed on the Signatures tab.

   a. Select the **Reason** that you wish to move the position of.

   b. Use the arrow keys on the right hand side of the list to move the **Reason** up or down as required.

   Repeat steps 1 to 6 for each Signature Point **Name**.

Defining the Same Settings for all Signature Points

1. To define the same settings for all Signature Points, click **Update All**.

   The Update All Signature Points dialog is displayed.

2. In the Require Signature section, select either **All Points require a signature**, **No Points require a signature**, or **Do not change the current settings**.

   If **Do not change the current settings** is selected, no change will be made to the **Require Signature** settings.

3. In the Prompt for comments, select either **All Points require a prompt**, **No Points require a prompt**, or **Do not change the current settings**.

   If **Do not change the current settings** is selected, no change will be made to the **Prompt for Comments** settings.

4. Click **OK**.

   The Update All Signatures dialog closes and the Signature Points dialog is re-displayed.

Passwords

During Login, users can be required to enter their **User name** and **Password**, or simply their User name. A password is not mandatory in Spectrum, but is mandatory in Spectrum ES.

1. From the Setup menu, select **Administration** and then click **Setup Users**.
2. The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.
3. Select the Password Control tab.
4. In the Login Type section, select:
    a. **PerkinElmer Login**, which requires the user to enter a User Name and Password.
    b. **No Passwords Login**, which requires the user to select their User Name from a drop-down list containing all Spectrum users (Spectrum Standard only).
    c. **Windows Login**, which requires that the PKIUsers group created during the installation of Spectrum has been populated by a Windows Administrator.

    See Windows Login.

NOTE: The No Passwords Login setting alters the behavior of the Login dialog. When selected, the user can select their user name from a drop-down list. When de-selected, the user must enter their user name manually because, for security reasons, a drop-down list is not available.

Changing or Setting a Password

NOTE: This procedure is applicable only when Login Type is set as PerkinElmer Login on the Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, change passwords using Windows User Management.

Changing your Password

You must change your password when prompted during login. This prompt occurs when an administrator mandates **User must change password at next login**, or when your password has expired.

You can also change your password during login, subject to the Minimum password age set for all users by an administrator.

1. At login, enter a valid **User name** and **Password**, and then click **Change Password**.

   The Change Password dialog opens.
2. Enter a **New password**, enter it again in the **Confirm password** field, and then click **OK**.
3. To complete the login, click **OK**.

NOTE: You can always change your password when prompted during login. However, you cannot then change your password before the Minimum password age set by an administrator for all users has expired. In Spectrum, the **Minimum password age: Allow changes after (days)** is set to 1, so if you attempt to change your password, the following message is displayed: 'You have changed your password less than 1 days ago. You cannot change your password again.' To allow passwords to be changed within the first day, an administrator must set **Minimum password age: Allow Changes Immediately**.

To Set a new Password (Administrator only)

An administrator can set a new password for a user unable to login because their password is lost or forgotten:

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.
2. On the Users tab, select the user from the **Name** drop-down list, then click **Edit**.

   The Edit User dialog is displayed.
3. Enter a new **Password** and then enter the password again in the **Confirm password** entry field.

   NOTE: Passwords are case sensitive, and can consist of letters, numbers and single spaces only.
4. Select **Enabled** if you wish the user to be able to login straightaway, or **Disabled** if you wish to enable the login later.

5. If **Enabled** is selected, select whether the **User must change password at next login**.
6. Click **OK**.

   The new password is implemented.

Maximum and Minimum Password Age

NOTE: These topics are only applicable when Login Type is set as PerkinElmer Login on the Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, administer passwords using Windows User Management.

NOTE: The settings on the Password Control tab apply to all users. It is not possible to define individual Password Controls for each user.

Maximum Password Age

On the Password Control tab, Maximum password age defines the maximum number of days that users can retain the same password before they must change it. By default the password expires after 42 days. The minimum is 1 day and the maximum is 999 days.

The Maximum password age cannot be set less than or equal to the Minimum password age.

NOTE: If you want to set the Maximum password age to 1 day the Minimum password age must be set to Allow changes immediately.

If it is not necessary for users to change their password, select **Password never expires**.

Minimum Password Age

On the Password Control tab, Minimum password age defines the number of days that users must retain the same password before being allowed to change it. The default setting for **Allow changes after (days)** is 1. Setting Allow changes after (days) prevents users from changing their password several times in a short space of time in order to return to a previous password.

To allow users to change their password immediately, select **Allow changes immediately**.

The Minimum password age cannot be set greater than or equal to the Maximum password age. The minimum is 1 day and the maximum is 999 days.

NOTE: If you want to set the Maximum password age to 1 day the Minimum password age must be set to Allow changes immediately.

Password Length

NOTE: These topics are only applicable when Login Type is set as PerkinElmer Login on the Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, administer passwords using Windows User Management.

Minimum password length on the Password Control tab defines the minimum number of characters that must be used in the password. By default, the **At least (characters)** setting is 6. The minimum setting is 1 character, and the maximum is 16 characters.

Allow blank password (Spectrum Standard only) means that users who have never logged in before (or who opted not to enter a password when they last changed their password) are not required to enter a password at login. In Spectrum ES, Allow blank password is not available as entering a password is mandatory.

NOTE: If a blank password expires (the Maximum password age setting is not **Password never expires**), a second blank password cannot be used immediately unless the Password uniqueness setting is **Do not keep a password History**.

Re-Using Passwords

NOTE: These topics are only applicable when Login Type is set as PerkinElmer Login on the Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, administer passwords using Windows User Management.

Password Uniqueness

Password uniqueness on the Password Control tab defines the number of new passwords that must be used before a previous password can be reused. For example, if the first password is 'spectrumid', and Number of passwords to remember is set to 24 (the default setting), a user must use 24 other passwords (in addition to their current password) before being able to use 'spectrumid' again.

The minimum **Number of passwords to remember** is 1 and the maximum is 24.

An additional Password uniqueness setting is Do not keep a password history, where no record of previous passwords is kept.

Password Records

By default, a record of previous passwords is made automatically.

Changes to passwords are logged. However the actual passwords are not visible; the word Hidden is displayed instead.

Select **Do not keep password history** (Spectrum Standard only) if you do not wish to retain a record of the number of previous passwords.

Password Lockout

NOTE: These topics are only applicable when Login Type is set as PerkinElmer Login on Password Control tab of the Users and Password Control dialog. When Login Type is set as Windows Login, administer passwords using Windows User Management.

Limiting failed Login attempts using Lockout

This procedures enables you to lock out a user that persistently fails to log in correctly.

1. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.

2. Select the Password Control tab.
3. Click **Account Lockout**.

   The Account Lockout dialog is displayed.

4. Enter the **Number of failed logins allowed before lockout**.

   For example, if Number of failed logins allowed before lockout is set to 5 (the default value), the user is locked out on their fifth failed attempt until an administrator allows them access again (Permanent) or for a specified period of time (Duration).

   The minimum number of failed login attempts before a user is locked out is 1. The maximum number of allowed failed login attempts before a user is locked out is 10.

   NOTE: If Number of failed logins allowed before lockout is 1, then the user is locked out after their first incorrect login attempt. That is, an incorrect login attempt is not allowed; the user must login successfully at their first attempt or be locked out.

5. Select the Lockout Duration as **Permanent, until administrator unlocks**, or **Duration (minutes)**. If you select Duration, enter the time (in minutes) for the lockout.

   Permanent means that the user will be unable to login again until an administrator has assigned a new password. Duration is grayed if Permanent is selected.

   Duration prevents the user being able to login again until the time specified has elapsed. If Duration is selected, the default is 60 minutes. The minimum Duration is 1 minute and the maximum Duration is 32767 minutes (22.75 days).

NOTE: Details of failed login attempts are recorded in the Login History.

Reinstating Locked Out Users

If Account Lockout is set to Permanent until Administrator unlocks and the user has failed to login correctly within the allowed number of attempts, an administrator must assign a new password before the user is able to login again.

If one or more users a has been locked out, when an administrator next logs in a list of Locked Out Users is displayed.

1. Highlight the name of the user that you wish to reinstate and then click **Edit**.

   The Edit User dialog is displayed.

   NOTE: If you click **OK** (rather than **Edit**) when the list of Locked Out Users is displayed, the list is closed. Any locked out users will remain locked out. The list will be re-displayed each time you log in until all locked out users have been assigned a new password.

2. Enter a new Password and repeat it in the Confirm password field.
3. Click **OK**.

   The user is removed from the list of Locked Out Users.

4. Click **OK** to close the Locked Out Users dialog.

   The previously locked out user will now be able to log in using the new password.

   You can mandate a password change by selecting User must change password at next login.

NOTE: In Spectrum ES **User must change password at next login** is mandatory.

Users locked out for a specified duration can be unlocked by the administrator in the same manner.

Windows Login

It is possible for users to log in to Spectrum using their Windows XP or Windows 7 User name and Password (instead of having a separate Spectrum User name and Password).

It is not possible to have some users that log in using their Windows User Name and Password while others use a separate Spectrum login.

NOTE: Being logged in as a Windows administrator gives full read/write permissions to the system. To avoid negating the 21 CFR Part 11 compliance, end users (that is, individuals using Spectrum ES software and instruments to collect data), should run as Windows Users, never as Windows administrators.

Adding Windows users to the PKIUsers group on a local PC:

To facilitate the use of Windows User names and Passwords, the PKIUsers group is created on the local PC during the installation of Spectrum. When Spectrum is installed and run on a local PC, the Windows administrator should add all the users who will access Spectrum to the PKIUsers group.

NOTE: When Spectrum is used across a network, the Windows administrator should create a network group on an accessible domain and then add users to that group.

1. Install Spectrum.
2. From the Windows Start menu select **Control Panel.**
3. Select **Administrative Tools** and then **Computer Management**.

   The Computer Management dialog is displayed.
4. Select **Local Users and Groups.**
5. Select the **Groups** folder to see the list of available Groups on the PC, and then double-click **PKIUsers**.

   The PKIUsers Properties dialog is displayed. The Members list already contains Everyone. This group has been created for folder access only, not as a Windows user group as it contains no user members.
6. To add a user member to the Group, click **Add**.

   The Select Users dialog is displayed.
7. To select a user from a different location (domain), click **Locations** and then select the required location for the user you wish to add.
8. To add a user to the group, enter the name of the user in the **Enter the object name to select** field and then click **Check Names**.

   Clicking Check Names will validate the name on the specified domain.

   NOTE: If you are not logged into this domain already, a login dialog will be displayed.

9. Click **OK**.

   The Select Users dialog is closed and the user is added as a member to the PKIUsers Properties dialog.

10. To add more users, repeat steps 6 to 9.

NOTE: It is possible to add a user more than once if they are on more than one domain as each Location together with the User name and Password will be unique.

All users added to the PKIUsers Group on the local PC, or added to a network users group, will be able to log in to Spectrum once a Spectrum administrator has defined the Login Type as Windows Login.

NOTE: Any users added to the PKIUsers Group before logging into Spectrum for the first time will appear in the Name drop-down list on the Users tab of the Users and Passwords Control dialog. If users are added subsequently, click **Update users** on the Users tab to refresh the Name drop-down list.

Defining the Spectrum Login Type as Windows Login:

The Login Type (Windows Login, PerkinElmer Login or No Passwords Login) applies to all users. It is not possible to have some users that log in using their Windows Login while others use a separate Spectrum login.

1. Start Spectrum and log in as an administrator.
2. From the Setup menu, select **Administration** and then click **Setup Users**.

   The Users and Passwords Control dialog (Spectrum) or the Users, Groups, Signatures and Password Control dialog (Spectrum ES) is displayed.
3. Select the Password Control tab.
4. From the Login Type drop-down list select Windows Login.

   All the other information previously displayed on the tab is removed as the password controls are now from Windows rather than Spectrum.

   The Load Windows Users dialog is displayed.
5. Select the **Domain** and specify the **Group** of Windows users that you wish to add to the list of Spectrum users.

   The default selection is the PKIUsers group on the local PC.
6. Click **OK**.

   The Windows users will be loaded and you may be prompted to select a new Spectrum administrator.

NOTE: If users are subsequently added to the PKIUsers group, to add these new Windows users to the list of Spectrum users a Spectrum administrator must click **Update users** on the User tab of the Users and Passwords Control dialog (Spectrum) or Users, Groups, Signatures and Passwords Control dialog (Spectrum ES).

To assign users Spectrum group memberships, see Assigning a User to a Group.

If a user is not added to at least one group, an error message will be displayed when they try to log in informing them that they do not have access to the application.

Logging in to Spectrum using a Windows Login

If you have been set up to log in to Spectrum using your Windows login:

1. Start Spectrum.

   (Select Start, All Programs, PerkinElmer Applications, Spectrum, and then Spectrum).
2. Enter your Windows User name and Password.
3. If the Log on to field is not displayed, click **Options**.
4. Select the required Domain from the Log on to drop-down list.

   By default, the Domain last logged on to is displayed.

NOTE: If all users are on the same Domain, there is no need to show the Log on to field as the correct Domain will be listed. To avoid confusion, this field can be hidden by clicking **Options<<**

Troubleshooting Windows Login

If you cannot login to Spectrum using your Windows Login, check that:

- Your Windows administrator has added your name to the PKIUsers Group.
- You have been assigned to at least one Group within Spectrum.
- You have entered the correct User Name and Password, and selected the correct Domain option from the Log on to drop-down list.
- PE21CFR is running. From the Start menu select Control Panel, and then select Administrative Tools. Then select Services. In the Services dialog check that PE21CFR is still running. If this has been paused or stopped you will be unable to login to Spectrum.

Password expiry

If whilst logging into Spectrum you get a message that your password is about to expire, you can change your password. This change applies to Windows as well as Spectrum.

Removing a User from the PKIUsers group in Windows:

1. From the Windows Start menu select **Control Panel.**
2. Select **Administrative Tools** and then **Computer Management**.

   The Computer Management dialog is displayed.
3. Double-click **Local Users and Groups**.
4. Double-click the **Groups** folder.

   The list of available Groups on the PC is displayed.

5. Double-click **PKIUsers.**

   The PKIUsers Properties dialog is displayed.

6. Select the appropriate user and then click **Remove.**

   The user is removed from the PKIUsers group.

Users Audit Trail (Spectrum Enhanced Security Only)

NOTE: The Users Audit Trail is available in Spectrum ES only. It can be viewed by members of the Administrators group only.

The Users Audit Trail records all changes to security settings in compliance with 21 CFR Part 11. All changes to users, groups and password settings are recorded. It also records when the Login History or Audit Trail have been exported and cleared.

1. Select **Users Audit Trail** from the Administration sub-menu of the Setup menu.

   The Login History, Audit Trail and Summary dialog is displayed.

2. Select the Audit Trail tab.

   The Audit Trail is displayed. For each change recorded, the following information is given in the Audit Trail:

   - **Function –** the item that was changed, for example, Add New User.
   - **Previous Value –** the state of the item before it was changed. Numbers refer to permissions or instruments; see Summary.
   - **Current Value –** the new state. Numbers refer to permissions or instruments; see Summary.
   - **Full Name –** the full name of the user who made the change.
   - **User Name –** the login user name of the user who made the change.
   - **Computer –** the name of the computer from which the change was made.
   - **Date Modified –** the date and time of the change.

Printing the Audit Trail

➢ To print the Audit Trail click **Print**.

All the information currently held in the Audit Trail is printed to the default printer.

Exporting the Audit Trail

1. To export the Audit Trail click **Export**.

   A Save As dialog is displayed.

2. Select the required destination and enter a filename.

   The Audit Trail is exported as a *.csv file that can be opened, for example, in Microsoft Excel.

Exporting the Audit Trail does not clear the Audit Trail entries from the dialog. However, you must export Audit Trail entries before they can be cleared.

Clearing the Audit Trail

➢ To clear the Audit Trail click **Clear Audit**.

You will be asked to confirm that you want to delete the Audit Trail log. All details are removed.

NOTE: It is only possible to clear Audit Trail entries that have previously been exported. If the Audit Trail contains additional entries since it was last exported, only those entries that have been exported will be deleted. If none of the entries have been

exported, a warning message will be displayed when you attempt to clear the Audit Trail.

Additional Information

The Users Audit Trail is saved to the Security database, Users.mdb.

The location of the security database is:

- Windows XP – C:\Documents and Settings\All Users\ Application Data\PerkinElmer\SecuritySystem\Users.mdb

  OR

- Windows 7/8 – C:\ProgramData\PerkinElmer\Securitysystem\Users.mdb

Login History (Spectrum Enhanced Security Only)

NOTE: The Users Audit Trail is available in Spectrum ES only. It can be viewed by members of the Administrators group only.

1. Select **Users Audit Trail** from the Administration sub-menu of the Setup menu.

   The Login History, Audit Trail and Summary dialog is displayed.

2. Select the Login History tab.

   The login history is displayed. This details every login attempt, since the history was last cleared, by:

   - **Full Name –** the full name of the user, or **Not Found** if the User Name entered did not exist.
   - **User Name –** the user name entered, whether correct or not.
   - **Computer –** the name of the computer
   - **Status – OK** indicates that the user logged in with the correct password; **Failed** indicates that a login was attempted with an incorrect password or User Name.
   - **Logged In –** date and time.
   - **Logged Out –** date and time.

Printing the Login History

- To print the Login History click **Print**.

All the information currently held in the Login History is printed to the default printer.

Exporting the Login History

1. To export the Login History click **Export**.

   A Save As dialog is displayed.

2. Select the required destination and enter a filename.

   The Login History is exported as a *.csv file and can be opened, for example, in Microsoft Excel.

NOTE: Exporting the Login History does not clear the Login History details from the dialog. However, you must export Login History entries before they can be cleared. See Clearing the Login History.

Clearing the Login History

- To clear the Login History, click **Clear History**.

  You will be asked to confirm that you want to delete the Login History log. All Login details are removed. The first Login details to appear after the Login has been cleared will be the date and time that you log out.

NOTE: It is only possible to clear Login History entries that have previously been exported. If the Login History contains additional entries since it was last exported, only those entries that have been exported will be deleted. If none of the entries have been exported, a warning message will be displayed when you attempt to clear the Login History.

The only limit to the size of the Login History is disk space, but we recommend that you review and archive it at regular intervals.

Summary (Spectrum Enhanced Security Only)

NOTE: The Users Audit Trail is available in Spectrum ES only. It can be viewed by members of the Administrators group only.

The document created by this command records a summary of the security status of the application.

1. Select **Setup Users Audit Trail** from the Administration sub-menu of the Setup menu.

   The Login History, Audit Trail and Summary dialog is displayed.

2. Select the Summary tab.

   The Summary records all information about the security settings:

   - **Application –** records the application for which this Summary applies.
   - **Password control** – records the Login type, Windows group, Maximum password age, Minimum password age, Minimum password length, Password uniqueness, Lockout count and Lockout duration settings.
   - **Permissions –** records the number of permissions, then lists each permission with a number that is used to identify the permission on the Users Audit Trail.
   - **Instruments –** records the number of instruments attached to the application. Each instrument is then listed with a number that is used to identify the instrument on the Users Audit Trail.
   - **Users –** records the number of users. It then records each User name, Full name, Status, Last Login, the Groups the user belongs to, the Permissions of that group and the Instruments the user has permission to use.
   - **Groups –** records the number of groups. For each Group it records the Group Name, the Users in the Group, the Permissions of that group and the Instruments the group has permission to use.

Printing the Summary

- To print the Summary click **Print**.

  All the information is printed.

Exporting the Summary

1. To export the Summary click **Export**.

   A Save As dialog is displayed.

2. Select the required destination and enter a filename.
3. Select to save the Summary as a *csv or as a *.txt file.
4. Click **Save**.

   The summary is exported as a *.csv file or *.txt file that can be opened, for example, in Microsoft Excel.

Assigning a New Group Workspace (Spectrum Enhanced Security Only)

A new workspace is created each time a user logs in to Spectrum (unless the user previously selected to reload their last workspace). By default, the new workspace is based on the software default workspace. However, members of the Administrators group in Spectrum can assign their current workspace as the default for a group.

Features that can be assigned to a group workspace include:

- Custom toolbars, reflecting the tasks frequently performed by a group of users
- Instrument Setups
- Sample Table Setups
- Macros
- Equations
- Software settings, such as Instrument settings; Instrument Performance Verification and Ready Checks settings; and Search, Compare and Quant parameters.

No spectra or data will be included in the default workspace.

Assigning the current workspace to existing groups

Before the workspace can be assigned as the default for a group, a user with the appropriate permissions should define the workspace, including toolbar layouts, Instrument Setups, Sample Table Setups, Macros and Equations.

To set the current workspace as the default for a group:

1. Log in to Spectrum as an administrator.
2. Set up the workspace you want to assign to a group or groups.

   Refer to Loading a Workspace to load an existing workspace.
3. From the Setup menu, select **Administration** and then **Set Group Workspace**.

   The Set Group Default Workspace dialog is displayed. The dialog lists all the groups in Spectrum.
4. Select the **Include** check box for the group(s) you want to assign the workspace to.
5. Click **OK**.

   The Sign Workspace dialog is displayed. The upper part of the dialog shows the Audit Trail. The lower part, if displayed, shows the signatures in the current workspace. To display the Signature Details list, ensure that **Show signature details** is selected.
6. To sign the workspace, click **Sign**.

   The Sign dialog is displayed.
7. Enter your **User name** and **Password**.
8. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

   NOTE: A reason will required if an administrator has defined Reasons on the Signatures tab for the Workspace signature point.
9. Enter any **Comment** required.

10. Click **OK**.

    The current workspace is saved as the new default workspace for the group(s) selected. The next time a new workspace is created on login by a member of that group, the new default will be used, unless that user is a member of more than one group. It will also be used if **Restore Default Workspace** is selected.

    If a user is a member of more than one group and one or more of those workspaces is modified, then the Choose Group Default Workspace dialog will prompt the user to select which group default to use to create a new workspace. This may be displayed when the user exits Spectrum and selects **Don't load spectra next time,** or when the user logs in to Spectrum.

Additional Information

User-defined objects

When a new group workspace is loaded, any user-defined objects such as Macros, Equations, Sample Table Setups and Instrument Setups are removed and replaced by the objects in the group workspace.

Common (Global) objects

When a new group workspace is loaded, any objects such as Macros, Equations, Sample Table Setups and Instrument Setups in the group workspace are loaded. Any objects in the appropriate common directory (defined during Spectrum installation) are also loaded. If any objects in the common directory have the same file name as an object in the workspace, then they are automatically renamed. For example, Macro 4 would be renamed as Macro 5.

Instruments

The Instruments sub menu of the Setup menu enables you to:

- Select an instrument from the list of available instruments, or Work Offline.
- Auto-Connect to a particular instrument.

Provided you are logged into Spectrum as an administrator, you can also:

- Add an instrument to the list of instruments available to Spectrum.
- Remove an instrument from the list of available instruments.

Add Instrument

Use the Add Instrument command to install an instrument and make it available to Spectrum (and to any other applicable PerkinElmer applications installed on this PC, such as AssureID).

You cannot add or remove an instrument unless you are logged into Spectrum as an administrator.

Add an FT-IR instrument

NOTE: If you have a Spectrum Two FT-IR/FT-NIR Spectrometer connected to the PC via the USB cable provided, an Ethernet cable or the optional PerkinElmer wireless router, the spectrometer will be detected automatically when Spectrum starts and added to the list of available instruments. You will only need to use the Instrument Install Wizard if you intend to connect your instrument using an Ethernet cable over a network.

1. Select **Instruments** from the Setup menu, and then click **Add Instrument**.

   The Install Instrument dialog is displayed.

2. Select **PerkinElmer FT-IR Instruments** from the drop-down list and then click **OK**.

   The Instrument Install Wizard is displayed. If you are currently connected to an instrument, it is disconnected until the wizard is closed.

3. Click **Next**.

   The Instrument Details page is displayed.

4. Enter the **Instrument Name**.

   This could be, for example, Spectrum Two FT-IR/FT-NIR, Frontier FT-IR, or any name to distinguish your instrument from another resource connected to the network.

5. Enter the **IP Address**.

   OR

   Click **Use Factory Default**.

   Make sure that the IP address you enter is compatible with the IP address scheme used by your network, and that the address is not used by an existing network resource, such as another PerkinElmer spectrometer.

6. Click **Next**.

   The Test Configuration page is displayed, and the connection and configuration for the instrument is checked.

   If any test fails you cannot proceed.

   For a Spectrum Two FT-IR/FT-NIR Spectrometer, when the configuration tests have passed, the Finish dialog is displayed. Continue at Step 8.

7. If the instrument has been installed on a previous occasion, so that the required instrument configuration file is available on your PC, click **Use Existing Configuration**.

   OR

   Insert the Configuration Files CD that was shipped with the instrument. Browse to the appropriate disk drive, highlight the configuration file and then click **Open**.

   When the configuration file has been copied from disk, the Instrument Configuration Disk dialog is closed and Completed is displayed at the bottom of the Test Configuration page.

8. Click **Next**.

   The Finished page is displayed, which enables you to examine the log file of any performance tests that have been performed.

9. Click **Finish**.

   The Instrument Install Wizard closes, the new instrument is added to the list of available instruments, and you are offered the opportunity to connect to the newly installed instrument.

10. Click **Yes** to disconnect from your current instrument (if applicable) and connect to the new instrument.

    OR

    Click **No** to reconnect with your current instrument (if applicable), or to work offline.

If you are adding an instrument that is used from other PCs, make sure that the Instrument service due in (days) and Desiccant change due in (days) values are correct.

Add a Raman instrument

1. Select **Instruments** from the Setup menu, and then click **Add Instrument**.

   The Install Instrument dialog is displayed.

2. Select **PerkinElmer Raman Instruments** from the drop-down list and then click **OK**.

   The Instrument Install Wizard is displayed.

3. Click **Next**.

   The Instrument Details page is displayed.

4. Enter an **Instrument Name**, which will be used by the Spectrum software to identify your instrument.

5. Click **Next**.

   The Copy Configuration Disk page is displayed, which prompts you to select the drive containing the configuration data. This data is shipped on a CD with your instrument.

6. Click **Next**.

   The Instrument Serial Number page is displayed.

7. Select your **Instrument Type** from the drop-down list.

8. Enter your instrument serial number and click **Next**.

   The Finished page is displayed.

9. Remove the configuration disk from the CD drive.
10. Click **Finish**.

    The Instrument Install Wizard closes, the new instrument is added to the list of available instruments, and you are offered the opportunity to connect to the newly installed instrument.
11. Click **Yes** to disconnect from your current instrument (if applicable) and connect to the new instrument.

    OR

    Click **No** to work offline.

Remove Instrument

Use the Remove Instrument command to delete an instrument from the list of instruments available to Spectrum and to any other applicable PerkinElmer applications installed on this PC, such as Spectrum or AssureID.

You cannot add or remove an instrument unless you are logged into Spectrum as an administrator.

1. Select **Instruments** from the Setup menu, and then click **Remove Instrument**.

   The Remove Instrument dialog is displayed.

2. Select the name of the instrument you want to remove from the drop-down list.

3. Click **OK**.

   A warning page is displayed. An additional warning is displayed if you select the instrument that is currently connected.

4. If you are certain that you want to delete this instrument from your system, click **Remove**.

   The instrument name is deleted from the list of instruments available.

   OR

   Click **Cancel** to exit close the Remove Instrument dialog.

Additional Information

It is not necessary to remove an instrument to select another instrument, or to disconnect the current instrument and work offline; use the Select Instrument command.

Select Instrument

Use the Select Instrument command to connect to an instrument if you are working offline, to free the current instrument and connect to another instrument, or to free the current instrument and work offline.

1. Select **Instruments** from the Setup menu, and then click **Select Instrument**.

   The Select Instrument dialog is displayed.

2. Select the name of the instrument you want to connect to from the drop-down list, and click **Connect**.

3. If the instrument is not available (disconnected, or in use by another user) a warning is displayed.

   OR

   Click **work offline**.

Additional Information

Always connect to this instrument

This option enables you to select this instrument connection as your Spectrum log in default. When selected, the Auto-Connect option in the Setup menu is enabled.

Managing the List of Available Instruments

If the instrument you want to connect to is not in the drop-down list of available instruments; see Add Instrument.

If the drop-down list of available instruments contains superfluous instrument connections; see Remove Instrument. If you have other PerkinElmer FT-IR software installed on your PC, remember that the instrument connection is removed from your system, not just the Spectrum software.

Auto-Connect

Use the auto-connect option to connect to a particular instrument automatically during log in, and skip the instrument connection dialog.

There are several ways to enable auto-connection to the instrument that is currently connected:

- Select the **Always connect to this instrument** check box in the Instrument Connection dialog during log in.

  This dialog will not be displayed if auto-connect is already enabled.

  OR

  Select the **Always connect to this instrument** check box in the Select Instrument dialog.

  OR

  Select the **Enable Auto-Connect** command from the Instruments sub menu of the Setup menu.

  When enabled, the auto-connect icon to the left of the command is highlighted in orange.

Setup Instrument

Use the Setup Instrument tabs to edit the settings used by your instrument, such as the initial values used in the Instrument Settings bar, or to restore the default settings.

- Select **Instrument** from the Setup menu.

  OR

  Select  in the **Setup** section of the Navigation Pane.

  The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

Setup Instrument - Basic	
Setup Instrument - Advanced	Toolbox
Setup Instrument - BeamPath	Desiccant
	Service
	Humidity
Setup Instrument - Data Collection	
Setup Instrument - Auto-Name	

Additional Information

The default settings used by Spectrum depend both on the type and configuration of the instrument, and any accessory fitted in its sample bay.

Spectrum remembers the settings last used for a particular configuration.

Setup Instrument - Basic

Use the Setup Instrument Basic tab to edit the settings used by your instrument, such as some of the initial values used in the Instrument Settings bar, or to restore the default settings.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

2. Select the Setup Instrument Basic tab.

Restore Defaults

Spectrum has a separate default instrument settings for each combination of instrument type, configuration and accessory.

For a particular combination of instrument type, configuration and accessory, Spectrum retains the settings used for the most recent scan. If you change instrument settings, but do not perform a scan, those changes are not retained.

To restore the system default instrument settings for the current combination of instrument type, configuration and accessory, click **Restore Defaults**.

Load and Save

You can save the current instrument settings, or load a previously saved set of instrument settings. To access the Instrument Settings dialog, click **Load and Save**.

The Instrument Settings dialog contains a list of Settings that have been saved. You can select a previously saved set of instrument settings and make these the current instrument settings that will be used to perform the next scan, using **Set as Current**.

The instrument settings list is specific to the User currently logged in to Spectrum. You can **Export** your instrument settings to a *.set file to be available to another user, or **Import** an existing *.set file (or secured *.sset file for Spectrum ES).

You can load settings that were created using a different instrument type, providing that the instrument settings are compatible. For example, you cannot load NIR instrument settings if you have an MIR instrument connected. A warning message will be displayed if the new settings are not allowed.

Instrument settings can also be loaded and used as part of a Macro.

NOTE: Instrument Setup files in Common Instrument Setups Directory will be visible to all users. The Common Instrument Setups directory is defined at Spectrum installation. The default is C:\pel_data\instrumentsetups

In Spectrum ES, Instrument Setups in the Common Instrument Setups Directory are added to the Instrument Settings dialog each time a new user workspace is created.

Signing, Reviewing or Approving an Instrument Setup (Spectrum ES only)

To Sign an Instrument Setup:

1. Select the row containing the Instrument Setup you want to sign for and then select **Sign** from the **Signatures** drop-down list.

   The Sign Instrument Setup dialog is displayed. This contains the Audit Trail entries for that Instrument Setup, and any signatures added previously.

2. To sign the Instrument Setup, click **Sign**.

   The Sign dialog is displayed.

3. Enter your **User name** and **Password**.

4. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

   NOTE: A reason will required if an administrator has defined Reasons on the Signatures tab for the Instrument Setup signature point.

5. Enter any **Comment** required.

6. Click **OK**.

   The Sign Instrument Setup entry is added to the Instrument Setup Audit Trail.

The Instrument Setup can now be exported for review or approval by a user with the appropriate permissions.

To Review or Approve an Instrument Setup:

Users with the appropriate permissions can import a signed Instrument Setup to review or approve it. The options **Review** and **Approve** then become available from the Signatures drop-down list. an Instrument Setup can be signed or reviewed more than once, and by more than one reviewer. A Instrument Setup can be approved without being reviewed, but once it has been approved it becomes read-only and can no longer be reviewed or edited.

1. Select the row containing the Instrument Setup you want to review or approve, and then select **Review or Approve** from the **Signatures** drop-down list.

   The Review Instrument Setup or Approve Instrument Setup dialog is displayed. This contains the Audit Trail entries for that Instrument Setup, and any signatures added previously.

2. To review or approve the workspace, click **Review** or **Approve**.

   The Review or Approve dialog is displayed.

3. Enter your **User name** and **Password**.

4. Select the appropriate pre-defined **Reason** from the drop-down list, if applicable.

> **NOTE:** A reason will required if an administrator has defined Reasons on the Signatures tab for the Review or Approve signature points.

5. Enter any **Comment** required.
6. Click **OK**.

   The Review Instrument Setup or Approve Instrument Setup entry is added to the Instrument Setup Audit.

The Instrument Setup can now be exported for review or approval by another user, if it has not been approved, or to be added to a group default workspace by an administrator.

Settings

<table>
<tr><td>Abscissa Units</td><td>
<table>
<tr><th>Units</th><th>Used</th></tr>
<tr><td>Wavenumber</td><td>The default unit for MIR spectroscopy.</td></tr>
<tr><td>Microns</td><td>The default unit for the Frontier Optica FT-IR and Spectrum 100 Optica FT-IR instruments.</td></tr>
</table>
</td></tr>
<tr><td>Ordinate Units</td><td>
<table>
<tr><th>Units</th><th>Used</th></tr>
<tr><td>%T</td><td>% Transmittance, used for qualitative analysis because small peaks are easier to see.</td></tr>
<tr><td>A</td><td>Absorbance, used for quantitative analysis because peak height is proportional to concentration.</td></tr>
<tr><td>%R</td><td>% Reflectance, used for reflectance spectra; numerically identical to %T.</td></tr>
<tr><td>log (1/R)</td><td>Log (1/Reflectance), used for diffuse reflectance spectra.</td></tr>
<tr><td>K-M</td><td>Kubelka–Munk units, used for diffuse reflectance spectra.</td></tr>
<tr><td>EGY</td><td>Energy, traditionally used for background spectra.</td></tr>
<tr><td>PAS</td><td>Photo-acoustic detector units.</td></tr>
<tr><td>ArbY</td><td>Arbitrary Y (ordinate) units, used for single-beam spectra in preference to EGY.</td></tr>
</table>
</td></tr>
<tr><td>Start</td><td rowspan="2">Set the scan range to the area of the spectrum that you are interested in, in wavenumbers (cm^{-1}). In this scale, the Start value must be greater than the End value.
The effective scan range that your instrument can collect depends on its configuration, including the detector and beamsplitter fitted, and also by the Scan Speed you select.</td></tr>
<tr><td>End</td></tr>
</table>

Scan Settings

Scan Type

Type	Use
Background	Used to collect a background spectrum to ratio against a sample spectrum.
Interferogram	Used to display the raw interferogram.
Interleaved	Only available when the sample shuttle accessory or NIRA II/NIRM is fitted. Automatically moves the shuttle to the rear position to take a background scan before moving to the front position to scan the sample and display a ratioed sample spectrum.
Sample	Used to collect a sample spectrum to automatically ratio against the current background spectrum.
Single Beam	Used to collect a sample spectrum that is not ratioed against a background spectrum.
Raw Interferrogram	Used in PerkinElmer collaboration. No direct functional use.

Resolution

Data Interval

Spectral resolution describes the ability of the instrument to distinguish between adjacent features in the spectrum. In effect, it defines the pathlength difference moved by the interferometer; the greater the pathlength difference the greater the wavelength precision. The spectral resolution value represents the smallest resolvable wavelength interval, so the smaller the value, the higher the resolution, and the greater the ability to distinguish peaks. The data interval, or digital resolution, is the spacing between the data points on the X axis. By default, the Data Interval is set automatically based on the set Resolution:

Resolution (cm^{-1})	Data Interval (cm^{-1})
0.5 - 0.99	0.125
1.0 - 1.99	0.25
2.0 - 3.99	0.5
4.0 - 7.99	1.0
8.0 - 64	2.0

Accumulations	You can elect to perform a number of Scans or to scan for a specific period of time. Enter a Scan Time in whole minutes or seconds. If you want to scan for less than 1 minute (60 seconds), select a number of Scans instead.

Accessory

Use the Accessory section to enter values for settings that are specific to the accessory fitted in the instrument sample bay.

The first item is the name of the type of accessory, which is detected automatically. If applicable, select an appropriate accessory option Value from the drop-down list.

Depending on your selection, further items may be added, each with its own drop-down list of possible values.

NOTE: For the Spectrum 65 spectrometer, the accessory type is not detected automatically and must be selected from the **Accessory** drop-down list.

For example, specific settings for the standard Sampling accessory are Not Specified by default, but if you specify that a Liquid Cell is fitted, you can also specify the Material that is used for the cell, the pathlength of the cell, and the Sample Type. All this information is stored with the scan.

NOTE: Provided they are used to perform a scan, any entries in the Accessories section are retained, just like any other instrument setting.

Additional Information

Background Spectrum

Whenever a background spectrum is required, this is indicated on the Measurement Bar, both in the Prompts Display and by a 'background' flag on the Scan button.

- To collect the background spectrum, make sure the beam path is clear, and then click  .

  This background scan is not displayed in the Viewing Area, or made available in the Data Explorer.

- To collect a background spectrum that can be saved and processed in the same ways as a sample spectrum, set the **Scan Type** to Background and click  .

  Once the background scan has been completed, the Scan Type is reset to Sample.

Resolution

The resolution required depends on the physical nature of your sample and the information you want to extract from the spectrum. For collecting mid infrared spectra from solid and liquid samples a resolution of 8 cm^{-1} or 4 cm^{-1} is often suitable, but if your sample is a gas a resolution of 2 cm^{-1} may be needed (0.5 cm^{-1} if the gas sample contains very small molecules).

Higher resolution spectra take longer to collect and more scans must be taken to achieve the same signal-to-noise ratio.

If you are collecting ratio spectra, the background spectrum must be of a resolution equal to or better than the resolution of the sample spectra. If the current background is invalid for your new settings, Spectrum prompt for a valid background.

Number of Scans and Duration

If you collect too few scans your spectrum may be noisy (have a poor signal-to-noise ratio) and you may not be able to distinguish peaks from the noise. However, collecting more scans than you need takes extra time. As a guide, collect 16 scans from your sample and then inspect the spectrum to see if it is good enough for your purposes. You may need to increase the number of scans you collect if you are looking for small peaks, or if you are using an accessory that limits the amount of energy reaching the detector.

The signal-to-noise ratio improves as more scans are added to the spectrum because noise occurs at random; the peaks in the noise are therefore not additive as the scans are accumulated. Real peaks in the spectrum always occur at the same point on the abscissa, they are therefore additive as the scans accumulate, making them larger than the noise.

Setup Instrument - Advanced

Use the Setup Instrument Advanced tab to edit the less routine settings used by your instrument, access the instrument Adjustments Toolbox, or to setup the Quality Checks applied to your scans.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

2. Select the Setup Instrument Advanced tab.

Toolbox

Click **Toolbox** to access the Adjustments Toolbox, which enables you to access a selection of instrument adjustment tools.

If you have a Spectrum Two instrument, you can access the source, desiccant and window replacement wizards from here.

Advanced Settings

CO2/H2O	Select this option to apply CO2/H2O Suppression to your spectrum as it is collected. Spectrum uses a theoretical water vapor and carbon dioxide spectrum to proportionally subtract appropriate bands from the gathered spectrum.
AVI	Select this option to apply AVI Correction to your spectra as they are collected. A perfect methane spectrum is compared with a methane spectrum gathered from a methane cell, which measures the instrument response. After this AVI Calibration, subsequently gathered spectra are corrected for this instrument response. This ensures wavelength accuracy and spectral data that is independent of the instrument used.
Look Ahead	Select this option to decrease overall scanning time using Look Ahead mode. In this mode, the instrument continuously gathers spectra using the current instrument settings, so can answer data requests more quickly.
Scan Speed (cm/s)	Scan Speed. Too slow a scan speed increases noise in the spectrum; too high a scan speed reduces the detected signal.
Phase Correction	Theoretical interferograms are perfectly symmetric in both branches from the centerburst. In the real world instrument imperfections and the necessary analog-to-digital conversion give rise to asymmetry in the digital

interferogram. Phase Correction measures the asymmetry of the gathered interferogram and tries to correct for it. The types of phase correction available are:

Type	Use
Self	Tries to estimate the interferogram asymmetry by analyzing the gathered interferogram itself. Therefore, the quality of the estimate depends on the quality of the gathered interferogram. This correction is useful for most samples, except when the gathered spectrum is noisy or very weak.
Background	Applies the phase correction of the background interferogram to the sample interferogram. This is most useful for samples that strongly absorb infrared radiation.
Magnitude	Corrects by calculating the RMS values of the Fourier transform wave elements. It cannot be used for a spectral resolution better than 2 cm^{-1}. If you use magnitude phase correction, it must be applied to both the background and sample spectra.
Previous	Applies the phase correction determined for the previous interferogram to the next interferogram gathered. This option assumes that the factors contributing to the asymmetry have not changed.

Apodization

A perfect interferogram would be infinitely wide. In practice the width of an interferogram is limited by its path difference so is always truncated at the end of each branch. Applying a Fourier transform to a truncated interferogram introduces ringing in the spectrum which is visible as sidelobes. Apodization applies a smooth roll-off function to the truncated ends of the gathered interferogram, which reduces the sidelobes and overall noise in your spectrum. However, depending on the function applied, spectral information may be lost, which broadens spectral features. If you are looking for narrow features, use a weak Apodization, or none. If you are looking for weak bands next to strong bands, use a strong Apodization to remove the sidelobes from the interferogram.

The types of Apodization available are:

Type	Use
Filler	Use when a very strong apodization function is required.
Strong	A strong Norton-Beer apodization function.

	Medium	A medium Norton-Beer apodization function.
	Weak	A weak Norton-Beer apodization function.
	Hamming	Used in PerkinElmer collaboration. No direct functional use.
	None, or 'Boxcar'	Use when the highest possible resolution is required. All points in the interferogra the resolution is not better than the smallest line width in the spectrum, sidelobe either side of the peaks.
Scan Start Delay	If you see a short delay between placing a sample in the beam and the generation of a wholly representative scan by the instrument, enter a Scan Start Delay (in seconds).	
Quality Checks	Quality Checks enable you to quickly identify potential problems with your spectra. Select the Quality Checks that you want performed as your spectra are collected and adjust the threshold **Range** using the slider controls. If you are very experienced, you may decide to click **All Checks Off** and not perform any checks. To select a comprehensive set of Quality Checks, click **Restore Defaults**.	

Additional Information

CO2/H2O Suppression

When CO2/H2O suppression is active, the software uses the theoretical spectra of water vapor and carbon dioxide to generate a model spectrum for the current conditions by least squares fitting to the current spectrum. This model spectrum overcomes non-linearity due to resolution, the temperature dependence of the measured spectrum, and the effects on lineshape and calibration by J-Stop and accessory vignetting. The water vapor and carbon dioxide bands are then removed from the measured spectrum.

CO2/H2O suppression will not be available in the FIR range.

AVI Correction

NOTE: AVI Correction requires an AVI Calibration to be performed for the current sampling configuration.

The objectives of the Absolute Virtual Instrument (AVI) correction routine are to provide consistent performance over time and between instruments, and traceability for all measurements.

Although FT-IR spectrometers use a reference laser, the wavenumber calibration and lineshape are affected in all FT-IR spectrometers by differences in beam divergence and uniformity. Differences can occur between instruments when using different sampling accessories and when instrument components are changed. AVI calibration ensures that wavenumber and lineshape are independent of the instrument used.

The Absolute Virtual Instrument is an instrument with theoretical performance, such that the result of measuring a known sample on such an instrument can be predicted. So, if we measure with a real instrument and calculate the software transform to match the theoretical result, we can apply this transform to future measurements. The Absolute Instrument is defined by wavenumber calibration, instrument lineshape and ordinate accuracy.

AVI corrects the performance of your instrument to an absolute standard, namely the spectrum from a methane cell. If a methane cell is fitted in the filter wheel, this will automatically be used for the AVI correction. The use of an on-board methane cell means that the correction can be applied for any sampling configuration. If your instrument does not have a methane cell installed, you will be prompted to insert a methane cell in the sample compartment. AVI will not be possible if your sampling accessory does not allow you to insert a methane cell.

AVI will not be available in the FIR range.

Look Ahead

In Look Ahead mode the spectrometer scans continuously and uses the properties of the measured spectrum to identify changes corresponding to sample removal, sample insertion, or sample change. By identifying the scans that are being collected, the software can accumulate sample scans and update background scans automatically.

When you request a sample scan the software checks back to identify a relevant background spectrum and looks to see whether it has already collected spectra belonging to the current sample. If it has, then not only is a background not required, but the number of scans requested is decreased by the number of scans already collected, so that the overall scanning time is decreased.

Look Ahead will not be available in the FIR range.

Scan Speed

Scan speed, for an interferogram, is the rate at which the optical path difference (OPD) is varied. The OPD is the difference in optical path between the two beams of the interferometer.

The default scan speed depends on the type of detector you are using:

Detector	**Default Scan Speed (cm/s)**
TGS	0.2
FIR TGS	1.0
Lithium Tantalate ($LiTaO_3$)	0.2
MCT	1.0
Photoacoustic (PAS)	0.2
InGaAs	1.0
InGaAs (NB)	0.2

These settings are the optimum scan speeds for the detectors to give the best signal-to-noise ratio in a reasonable collection time.

For a TGS or Lithium Tantalate detector, increasing the scan speed results in a lower signal-to-noise ratio. This decrease in signal-to-noise ratio is not offset by increasing the number of scans collected to maintain the overall collection time.

An MCT detector gives a better signal-to-noise ratio at higher scan speeds for a given overall collection time.

NOTE: The scan range upper limit may be reset to one of two values when you change the scan speed.

These values are: 15 000 cm^{-1} for a scan speed of less than or equal to 1 cm/s; 7800 cm^{-1} for a scan speed of 2 cm/s.

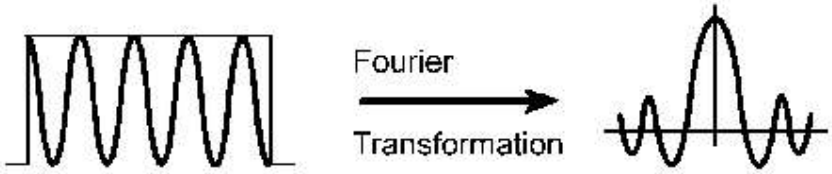
Phase Correction

An ideal interferometer would produce an interferogram that was totally symmetrical about its center. No interferometer produces an ideal interferogram.

The phase correction step in processing an interferogram can be avoided by calculating the magnitude spectrum. Magnitude spectra are not affected by phase errors but are subject to ordinate errors in regions of low transmittance and give photometric errors for highly absorbing bands.

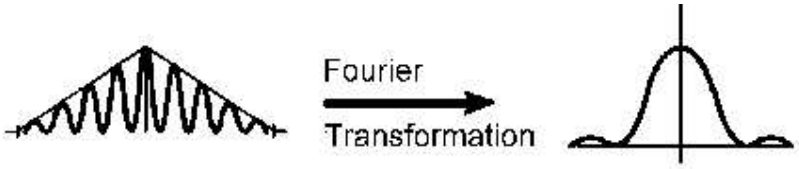
Apodization

An FT-IR spectrometer generates an interferogram by scanning a moving mirror over a finite distance. However, if no information is to be lost, the interferogram must extend between plus and minus infinity. Stopping the mirror truncates the interferogram and limits the resolution, as if the interferogram had been multiplied by a "boxcar" function.



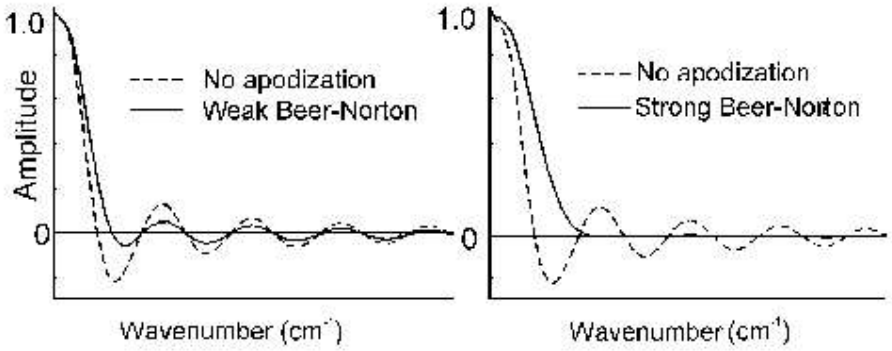
This boxcar truncation introduces lobes (or 'feet') at the sides of the peak. These lobes are a result of the abrupt end of the data collection.

Apodization is the mathematical process used to remove these lobes (apodization is from the Greek 'apod', meaning 'without feet'). One way to remove these feet is to use a Triangular apodization, which gives less weight to the data away from the center of the interferogram.



Although the feet are smaller, the peak is broader. When a spectrum is apodized, the full width at half height (FWHH) of the peak can be up to twice as large as the FWHH of the unapodized peak.

There are many different apodization functions, each of which tries to find the best compromise between removing the feet and limiting the peak broadening. You can choose weak or strong Beer-Norton apodization, or no apodization at all (Boxcar). The figure below shows the effect of both weak and strong Beer-Norton apodization, compared to a band with no apodization. Strong Beer-Norton apodization eliminates the artifacts completely in this case, but broadens the band more than does weak Beer-Norton apodization.



For most applications, the strong Beer-Norton apodization function is the most appropriate. For gas-phase samples, you can get a higher resolution by using a weak Beer-Norton but, to avoid losing spectral detail in the ripples, you must make sure that the spectrum has strong absorption lines.

Quality Checks

A Quality Check looks at a property of your spectrum during data collection and applies a status flag: Green (when your spectrum appears to be OK), Yellow (when it may be possible to improve the quality of your spectrum), or Red (when there is a serious problem with the spectrum).

Quality Checks settings are defined for the particular combination of instrument type, configuration and accessory. Spectrum retains the settings used for the most recent scan.

For more information about a particular Quality Check, and suggestions for ways to improve the measurement, double-click on its name in the list on the Advanced Instrument Setup tab.

Quality Checks will not be available in the FIR range.

All Quality Checks are set to off by default when you are connected to a Spotlight 150 microscope.

Adjustments Toolbox

Use the Adjustments Toolbox to access a selection of instrument adjustment dialogs.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the Setup section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

2. Select the Setup Instrument Advanced tab and then click **Toolbox**.

   The Adjustments Toolbox dialog is displayed:

	WCal	Adjust the wavelength calibration for your instrument.
	Align	Align your instrument.
	Center Burst	Find the position of the center burst for your instrument.
	AVI Calib	Perform an AVI calibration for the current instrument scan parameters.
	Instrument Display	Change the contrast settings on your instrument display.
	Fiber Probe Display	Change the brightness and contrast settings on your NIR Fiber Optic Probe display.
	Windows Replacement Wizard	Change your instrument sample area windows.
	Desiccant Replacement Wizard	Change your instrument desiccant.
	Source Replacement Wizard	Change your instrument source.
	Reference Correction	Standardize a reference material for the NIRA II/NIRM accessory.
	Stray Light Correction	Correct for stray light in the NIRA II/NIRM accessory.

3. Click on the tool for the adjustment you want to make.

   The appropriate tool dialog is displayed.

4. When you have finished, click **Exit** to close the Adjustments Toolbox.

Additional Information

- The Instrument Display tool is only available when connected to Frontier IR, Spectrum 100 Series or Spectrum 400 series spectrometers.
- The Fiber Probe Display tool is only available when an NIR Fiber Optic Probe sampling accessory is fitted.
- Windows, Source and Desiccant Replacement Wizards are only available for the Spectrum Two FT-IR/FT-NIR spectrometers. Each option displays a Wizard that guides you through the procedure for replacing these parts. Follow the instructions on-screen.
- The Reference Correction and Stray Light Correction are only available when a NIRA II/NIRM accessory is fitted. Each option displays a Wizard that guides you through the procedure for collecting the appropriate correction spectra. Follow the instructions on-screen.

Wavenumber Calibration

Use the Wavenumber Calibration tool, in conjunction with a recent reference spectrum collected by the instrument, to apply a corrective shift to the wavenumber scale.

You can collect a suitable reference spectrum using either the polystyrene sample supplied in the filter wheel of your instrument, or if your instrument does not have an internal, automated filter wheel, using a polystyrene sample inserted in the sample compartment. These samples are 'traceable at source'.

NOTE: A wavenumber shift may be the result of sample effects. When the wavenumber calibration is redefined, take care when comparing spectra with previously-collected spectra, library spectra, or when performing instrument validation due to minor shifts in peak positions.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

   NOTE: To see the tabs, you may have to resize the Dialog Pane.

1. Select the **Setup Instrument Advanced** tab and then click **Toolbox**.

   The Adjustments Toolbox dialog is displayed.

2. Click  .

   The Wavenumber calibration dialog is displayed.

3. Make sure that the **Calibrate from known band** option is selected.
4. Enter the expected position of a band in cm^{-1} in the **Expected position** text box.
5. Use a 35 µm polystyrene sample and the 3060.14 cm^{-1} band for a mid-IR instrument.

   OR

   Use a 1.4 mm polystyrene sample and the 5669.3 cm^{-1} band for an NIR instrument.

6. Enter the observed position of that band in cm^{-1} in the **Observed Position** text box.
7. In the **Apply calibration to configuration** section, select the appropriate wavelength range and accessory from the **Configuration** drop-down list.

   For example, if you were using a polystyrene reference as suggested above, you would select MIR - All accessories. You can also calibrate your system for when you are using the instrument with a number of specific NIR accessories. The available options include NIR - Reflectance (NIRA II/NIRM), NIR - Reflectance (NIRA II/NIRM) external, NIR Fiber probe (triggered), NIR Fiber probe (passive), and NIR - Other accessories. The current configuration is indicated by a *.

8. Click **OK**.
9. If the error message **Laser Wavenumber > 1% from nominal value** is displayed, which is very unlikely, check the validity of this message by making sure that the values entered in the **Observed Position** and **Expected Position** text boxes are correct.

a. If the error message **Laser Wavenumber > 1% from nominal value** is valid, so that a correction to the HeNe wavenumber greater than 1% is required:

b. Click **Set laser wavenumber**, and then click **Reset** to set the laser to its default nominal value.

c. Collect a new reference spectrum using your polystyrene TRM and repeat the calibration.

   If a correction greater than 1% is still required, you can enter a new laser wavenumber using this dialog, and repeat the calibration using your polystyrene TRM.

d. If a correction greater than 1% is still required, contact your PerkinElmer Service Engineer.

10. Click **OK.**

    The value of the Laser Wavenumber in the instrument is reset.

11. If you want to check the Laser Wavenumber, open the dialog again, check the stored value and then close the dialog.

12. Click **Exit** to close the Adjustments Toolbox.

Additional Information

Wavenumber calibration is controlled by the value of the stored HeNe laser wavenumber. You can adjust this calibration by up to 1% (158 cm^{-1}) of the nominal HeNe value by entering the expected and observed positions of a carefully selected reference peak in the Wavenumber Calibration Tool, which utilizes the relationship:

$$\frac{\text{CorrectedSpectrometerLaserWavenumber}}{\text{CurrentSpectrometerLaserWavenumber}} = \frac{\text{ExpectedBandWavenumber}}{\text{ObservedBandWavenumber}}$$

Changing the HeNe laser wavenumber only affects the interpolation of data collected subsequently. You cannot make the laser wavenumber different for sample and background spectra.

Traceable Reference Material

You may prefer to keep your own sample of Traceable Reference Material (TRM). A suitable sample of polystyrene TRM (35 µm for mid-IR, 1.4 mm for near-IR) is supplied with the Instrument Performance Verification (IPV) Kit for your instrument.

Using an external TRM sample, such as from the appropriate IPV Kit, enables you to validate the wavenumber calibration against NIST (National Institute for Standards Technology) standards.

Align

Use the Align tool to align the instrument with the position of the interferogram center burst.

1. Allow the temperature in the optical module to stabilize.

   This may be required if the instrument was switched off (or in Power Save mode), or if you have changed range on a dual-range instrument. Allow approximately 30 minutes.

2. Make sure that the sample compartment is empty.

3. Select **Instrument** from the Setup menu.

   OR

   Select  in the Setup section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

4. Select the **Setup Instrument Advanced** tab and then click **Toolbox**.

   The Adjustments Toolbox dialog is displayed.

5. Click  .

   The Instrument Alignment dialog is displayed.

   Alignment of the instrument begins.

CAUTION:	Do not disturb the instrument during the alignment process by, for example, obstructing the infrared beam in the sample compartment. If significant absorption occurs in the sample area, the beam energy reaching the detector may not be sufficient to allow alignment.

6. When alignment is complete, click **OK**.

7. Click **Exit** to close the Adjustments Toolbox.

Center Burst

Use the Center Burst tool to locate the position of the center burst.

NOTE:	This tool is primarily for use by Service Engineers.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

2. Select the **Setup Instrument Advanced** tab and then click **Toolbox**.

   The Adjustments Toolbox dialog is displayed.

3. Click  .

   The center burst is relocated.

   To stop the process before completion, click **Cancel**.

4. When the process is complete, click **OK**.
5. Click **Exit** to close the Adjustments Toolbox.

Additional Information

At the center burst, the scanning mirrors in the interferometer are positioned such that there is zero path difference between the two beams when they recombine. At this point, the infrared radiation interferes constructively at all wavelengths, so the amplitude of the interferogram is at its maximum.

AVI Calibration

Use the AVI Calibration tool to set up the AVI correction needed for the current sampling configuration. You can then apply AVI Correction to your spectra as they are collected; see Setup Instrument Advanced.

NOTE: You can also start the AVI Calibration by clicking  on the Measurement bar, if displayed, or by selecting **Standardize** from the Measurement menu.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

   NOTE: To see the tabs, you may have to resize the Dialog Pane.

2. Select the **Setup Instrument Advanced** tab and then click **Toolbox**.

   The Adjustments Toolbox dialog is displayed.

3. Click  .

   The AVI calibration routine begins.

4. Make sure that the sample area is clear and nothing is blocking the beam, and then click **Continue**.

   The background spectrum is collected.

   If you have a filter wheel with a methane cell installed, the AVI calibration will continue to collect a spectrum of the methane cell. Continue at Step 6.

5. If you do not have a filter wheel, or your filter wheel does not contain a methane cell, insert a methane cell in the sample beam, and then click **Continue**.

   The methane spectrum is collected.

6. When the calibration is complete, click **OK** in the confirmation dialog.

7. Click **Exit** to close the Adjustments Toolbox.

Additional Information

The Absolute Virtual Instrument (AVI) feature corrects the performance of your instrument to an absolute standard, namely the spectrum from a methane cell. In instruments where a methane cell is fitted in the filter wheel, the AVI calibration can be applied to any sampling configuration.

Instrument Display

Use the Instrument Display tool to adjust the Contrast of the Instrument Display on a Frontier IR, Spectrum 100 Series or 400 Series spectrometer.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

2. Select the **Setup Instrument Advanced** tab and then click **Toolbox**.

   The Adjustments Toolbox dialog is displayed.

3. Click  .

   The Display Settings dialog is displayed.

4. Adjust the Display Contrast to suit your working environment and then click **OK**.

   The Display Settings dialog closes.

5. Click **Exit** to close the Adjustments Toolbox.

Fiber Probe Display

Use the Fiber Probe Display tool to adjust the Brightness and Contrast of the display on an NIR Fiber Optic Probe connected to a Spectrum Two FT-NIR, Frontier IR, Spectrum 100 series or Spectrum 400 series spectrometer.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

2. Select the **Setup Instrument Advanced** tab and then click **Toolbox**.

   The Adjustments Toolbox dialog is displayed.

3. Click  .

   The Display Settings dialog is displayed.

4. Adjust the **Display Brightness** and **Contrast** to suit your working environment, and then click **OK**.

   The Display Settings dialog closes.

5. Click **Exit** to close the Adjustments Toolbox.

NIRA II/NIRM Corrections

The NIRA II/NIRM accessory features window, reference and stray light corrections to help ensure that its performance remains optimized throughout its service lifetime. These corrections are enabled from the Accessory section of the Setup Instrument Basic tab, and then automatically applied as spectra are collected. You can update the reference and stray light corrections if required using the wizards in the Adjustment Toolbox to collect new spectra.

NOTE: If you choose to apply any of the correction routines, they will be applied to all subsequent measurements on your system until you disable them.

Reference Correction

Diffuse reflectance spectra obtained from the NIRA II/NIRM are measured relative to a white reflector reference material. The NIRA II/NIRM is supplied with an internal sample of this reference material, or you can use your own external reference material placed over the sample window. The Reference Correction standardizes the chosen reference material against a separate standard, which ensures that reproducible results are obtained by different systems that use a NIRA II/NIRM.

The internal reference material is standardized against a standard maintained at the PerkinElmer factory. The corresponding correction spectrum should be copied on to your system when the NIRA II/NIRM accessory is installed, and should not normally need to be updated unless you purchase a new accessory. Alternatively, you can choose to standardize the internal reference material against your own external standard.

If you want to use an external reference material instead of the internal reference, it is also possible to standardize this external reference against an external standard. In this way, multiple NIRA II/NIRM systems, each with their own external references, can all be standardized against a common standard.

Stray Light Correction

Stray light is light from the instrument that reaches the detector without having interacted with the sample, which can cause distortion of strong absorptions in your spectrum. Although the NIRA II/NIRM has been designed to minimize stray light, some light scattering will always occur at the sample window, and this effect is increased if the window becomes dirty or scratched. The Stray Light Correction allows you to compensate for this unavoidable source of error in the spectrum.

This correction should only be updated if the stray light increases due to light scratching of the sample window. It should not be regarded as a substitute for keeping the window clean and avoiding creating scratches. If the stray light rises above a certain threshold, as indicated by a red line on the monitoring screen of the wizard, then the software can no longer adequately correct your results.

When you reach the monitoring screen of the Stray Light Correction Wizard, carefully clean the sample window. If the stray light spectrum is above the red line, the level is too high and the wizard will not allow you to collect a correction spectrum. You should close the wizard and investigate the problem. If further cleaning does not reduce the stray light sufficiently, then it is likely that a new sample window is required.

Windows Correction

The Window Correction compensates for the effect of the NIRA II/NIRM sample window by subtracting a reference spectrum measured at the PerkinElmer factory. If it is enabled, it will automatically be applied when appropriate, most commonly when the background spectrum is collected from the internal reference material and the sample is placed on the sample window.

For more information on the NIRA II/NIRM corrections, refer to the user's guide supplied with your accessory.

Applying the Corrections

1. Select **Instrument** from the Setup menu.

   The Setup Instrument Basic tab is displayed.

2. In the Accessory section, click the **Value** corresponding to the correction you want to apply.
3. Select **On** to apply the correction (or **Automatic** in the case of the Window Correction).

You can also select **Off** to stop applying the correction.

Setup Instrument - BeamPath

Use the Setup Instrument BeamPath tab to set up the beam path of your instrument, and to set up the components in the beam path.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

   NOTE: To see the tabs, you may have to resize the Dialog Pane.

2. Select the Setup Instrument BeamPath tab.

BeamPath Graphic

The graphic representation of the beam path in your instrument is redrawn to reflect any changes in the beam path, such as when you change the sampling accessory.

Click on a component in the beam path graphic to highlight a setting applicable to that component in the Settings Table.

Settings Table

The Settings table identifies the components in the beam path, such as the source, beamsplitter, detector, J-Stop, B-Stop, filter wheel, and sampling accessory, as applicable to your instrument. The Optimum Scan Range for the combination of source, beamsplitter and detector in the beam path is displayed.

If the Value for a Setting can only be changed by physically exchanging the component, the row is grayed. For example, the Settings table is updated whenever you change the sampling accessory.

If the Value for a Setting can be changed using the software, the row is highlighted in white. Select the value you want to change; in many cases a control is displayed to assist your selection of an appropriate value.

The options displayed in the table will depend on the instrument and accessory you are connected to. For example, if you are connected to a dual-range spectrometer, controls will be available to allow you to change the Mode. See Changing Mode.

If you have an external accessory installed, the Settings table will include the Beam Location. Direct the beam path to the accessory you wish to use by selecting **Front internal**, **Right external** or **Left external**, as required. The beam path graphic will be updated to show your selection.

NOTE: The default scan range will be updated for the instrument configuration.

If you have a Spotlight 150 and direct the beam path to the microscope, the controls on the Setup Microscope tab are enabled.

Additional Information

Warnings

Some settings may generate Warning flags both here and in the Status Bar:

- Instrument Service.
- Desiccant Change.
- Humidity Warning (Optional).

Changing Mode

If you are connected to a dual-range spectrometer, additional controls will be available in the Settings table to enable you to change between wavenumber ranges.

If you have a dual-range FT-IR/FT-NIR spectrometer you can choose between **MIR**, **NIR** and **Custom** modes. If you have a dual-range FT-IR/FT-FIR spectrometer, you can choose between **MIR**, **FIR** and **Custom** modes. If you select **Custom**, you can then change the Source, Beamsplitter and Detector independently. Some combinations, however, could damage the instrument, and will not be allowed.

If you change the **Mode** or modify the custom settings, click the **Apply** button to move the instrument hardware. If you have made a change that has not been applied yet, a message will be shown in the Prompts Display. Clicking Scan will apply the changes before collecting data.

If you change range, you may be prompted to change the sample compartment windows before applying the change.

Detector Ranges

Detector	Range (cm-1)
mid-IR TGS with KBr window	10 000 - 370
mid-IR TGS with CsI window	10 000 - 220
wide band MCT	10 000 - 450
medium band MCT	10 000 - 580
narrow band MCT	10 000 - 700
photoacoustic (PAS)	4000 - 400
Lithium Tantalate	10 000 - 370

NOTE: Refer to the *Spotlight 150 User's Guide* for details of the low wavenumber limits for the Spotlight 150 detectors.

Beamsplitter

A beamsplitter is a plate with approximately equal transmittance and reflectance; it is used to generate and recombine the two beams of the interferometer.

The choice of beamsplitter material depends upon the wavenumber range you want to study:

KBr and CsI beamsplitters are hygroscopic, and must be stored in desiccated boxes.

Beamsplitter	**Range (cm-1)**
CaF2	7800 - 1200
extended KBr	7800 - 370
KBr	7000 - 400
CsI	5000 - 220

J-Stop

A J-Stop (Jacquinot-stop) is an aperture in the beam path of the spectrometer. It is used to control the beam divergence in the instrument that arises as its spectral resolution is increased.

Automated internal J-Stop spectrometers

In instruments with an automated, internal J-stop a software-controlled iris sets an appropriate J-Stop Image Size for the current Resolution setting.

A smaller J-Stop Image Size restricts the amount of energy reaching the sample, so there may be occasions when a larger setting may be more appropriate.

However, a larger J-Stop Image Size limits the range to which a particular spectral resolution can be achieved, expressed by the **J-Stop Wavenumber**. You may prefer to set the J-Stop Image Size indirectly, by setting an appropriate J-Stop Wavenumber.

Fixed internal J-stop spectrometers

Some spectrometers (Spectrum Two, Spectrum 65) have a fixed, internal J-Stop. For operation at higher resolutions the J-Stop cards supplied can be inserted into the Sample Holder.

The current J-Stop Image Size is displayed in the Status Bar at the bottom of the workspace. If you change the **Resolution** (cm^{-1}), the J-Stop Image Size will be updated automatically. If you have a Sample Holder installed, a message will displayed on in the table, and in the Status Bar, asking you to insert one of the J-Stop cards, or to remove any external J-Stop card.

You can change the J-Stop Image Size (mm) independently of the Resolution. The options in the drop-down list will depend on your spectrometer. The J-Stop Wavenumber is defined for that Resolution and J-Stop Image Size.

NOTE: For accessories other than the Sample Holder, if you change to a Resolution higher than 2 cm^{-1} the scan range over which you can achieve that resolution will be reduced. Please refer to the J-Stop Wavenumber displayed in the table.

B-Stop

When you are connected to a Frontier Optica FT-IR or a Spectrum 100 Optica FT-IR spectrometer, the BeamPath Graphic and Settings Table includes the instrument's variable B-Stop.

A B-Stop (Baffle-Stop) is a variable iris that limits the divergence of the beam through the instrument. Stopping down (that is, reducing the size of) the B-Stop can improve the accuracy of your measurement at the expense of some sensitivity. For example, stopping down can reduce spurious attenuation or artifacts arising from unwanted reflections, but the signal-noise-ratio of your spectra may be lower.

- To override the default B-Stop setting, enter a new B-Stop Size in the Settings Table.

Filter Wheel

If you spectrometer has an automated, internal filter wheel, the BeamPath Graphic and Settings Table includes the Filter Wheel. You can select the filter in position in the beam path using the drop-down list in the settings table.

Placing a filter in the beam path enables you to optimize the system for a particular wavenumber range. For example, a filter can be used to facilitate the study of weakly absorbing samples. Reducing the wavenumber range allows more energy in the region of interest to reach the detector without saturating it. Thus, the signal-to-noise is improved in the specified wavenumber range.

The filter wheel includes the polystyrene and Schott NG11 glass filters used for validation procedures. It may also contain a methane cell for use in the AVI calibration.

Instructions for fitting new or replacement filters can be found in your instrument User's Guide.

Instrument Service

Use the **Instrument service due in (days)** Setting on the Setup Instrument Beam Path tab to view the number of days before the next instrument service, acknowledge that an instrument service has been performed, and to reset the number of days before the next instrument service.

This value is held locally on your PC. For a networked instrument, set this Value at each PC where the instrument is used. It can be helpful to nominate an individual to hold the service record for the instrument.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

2. Select the Setup Instrument BeamPath tab.

   Inspect the Value of the Instrument service due in (days) Setting. This counter decrements by 1 each day.

3. To reset the Instrument Service due in (days) counter, select its Value, click **Serviced** to clear any Warning messages, and enter the number of days before the next instrument service is due.

Additional Information

If an instrument service is overdue a warning is placed in the Status Bar and on the Setup Instrument BeamPath tab.

Desiccant Change

Use the **Desiccant change due in (days)** Setting on the Setup Instrument BeamPath tab to view when the next instrument desiccant change is due, acknowledge that the desiccant has been changed, and to reset the number of days before the next desiccant change.

For some instruments this setting is held locally on your PC. For a networked instrument, set this Value at each PC where the instrument is used. It can be helpful to nominate an individual to hold the service record for the instrument. However, for Spectrum Two instruments the desiccant change interval is held in the instrument's internal memory and is automatically downloaded to the PC on connection to the instrument.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see the tabs, you may have to resize the Dialog Pane.

2. Select the Setup Instrument BeamPath tab.

   Inspect the Value of the Desiccant change due in (days) Setting. This counter decrements by 1 each day.

3. To reset the Desiccant Change due in (days) counter, select its Value, click **Changed** to clear any Warning messages, and enter the number of days before the next desiccant change is due.

Additional Information

If an instrument desiccant change is overdue a warning is placed in the Status Bar and in the Setup Instrument BeamPath table.

Some PerkinElmer FT-IR spectrometers have a desiccant change indicator in the lid that should override any reminder set here. Change the desiccant when the sector marked 10 in the indicator has changed from blue to pink, and before the other sectors become pink.

The Spectrum Two spectrometer has an internal humidity sensor that reports the current humidity inside the instrument. Change the desiccant if the % humidity value reported in the Humidity Shield is displayed Yellow or Red. If the humidity is "high or at "danger" levels, a warning will be displayed in the Status bar.

Refer to the User's Guide for your instrument for information about how to change the desiccant packs.

NOTE:	If you have a Spectrum Two spectrometer, a Wizard is available to guide you through the desiccant replacement. Select Toolbox from the Setup Instrument Advanced tab and then click **Desiccant Replacement Wizard**.

Humidity Warning (Optional)

If a humidity warning message is displayed on the Status Bar by the optional humidity warning sensor:

1. Do not turn the instrument off.
2. Change the desiccant.

   Refer to the User's Guide for your instrument for information about how to change the desiccant packs. For the Spectrum Two spectrometer use the Desiccant Replacement Wizard.
3. Wait for half an hour to allow any fogging of the instrument optics to clear.
4. If your instrument has a desiccant indicator, wait until all the sectors in the desiccant indicator are blue. If you have a Spectrum Two spectrometer, wait until the value for the current internal humidity (%) displayed in the Humidity Shield dialog is green.
5. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE: To see the tabs, you may have to open, or resize, the Dialog Pane.

6. Select the Setup Instrument BeamPath tab.
7. Reset the Desiccant change due in (days) Setting.

   If you have a Spectrum Two Spectrometer, the desiccant change date will be updated automatically after the Wizard has finished.

Additional Information

Consider the humidity warning sensor option if your instrument is used in warm humid conditions, particularly if it is a mid-IR instrument.

The humidity sensor is available as standard on the Spectrum Two spectrometers and as an option for the Frontier IR systems, the Spectrum 100 and 400 Series spectrometers, and the Spectrum One and Spectrum One NTS spectrometers.

Setup Instrument - Data Collection

Use the Setup Instrument Data Collection tab to set the Auto-Save option, and to set whether to display the Live tab in the Viewing Area during data collection.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

   NOTE: To see the tabs, you may have to resize the Dialog Pane.

2. Select the Setup Instrument Data Collection tab.

Background Options

By default, you are not prompted to collect a new background spectrum unless none has been collected; you have changed the sampling accessory; you have applied an instrument setting that invalidates the background scan (such as a higher resolution or scan speed); or a new background is required by the instrument for some other reason.

If, for example, the Standard Operating Procedures (SOPs) for your laboratory require you to collect a new background spectrum at a specified interval, select the appropriate Background Option, and then enter a number of samples (10, by default), or an elapsed time (60 minutes, by default).

Auto-Save Options

Select **Save after each measurement** to automatically save each spectrum as it is collected, and then define the **Save Location** for all spectra. The default is C:\pel_data\spectra. Deselect this option if you want to explicitly select the spectra you want to save yourself.

NOTE: If you modify the default Save Location on the Setup Instrument Data Collection tab, then the Save Location on the Sample Table tab is also updated. In Spectrum ES if you do not have the appropriate permission, then you will not be able to modify the Save Location.

NOTE: In Spectrum ES, spectra are not saved to disk until the workspace is signed.

Select **Export** to automatically save each spectrum to the **File Format** selected in the drop-down lists. Then define the **Save Export Location**. The default Save Export Location is C:\pel_data\export. Deselect this option if you want to explicitly select the spectra you want to export yourself.

The File Formats available are Comma Separated Values (.csv), JCAMP-DX (.DX), ASCII (.ASC) and Custom Defined Format.

Comma Separated Value (*.csv) is a common file format that can be read into, for example, a Microsoft Excel spreadsheet or a Laboratory Information Management System (LIMS). JCAMP-DX (*.DX) is a standard file format for spectral data specified by the International Union of Pure and Applied Chemistry (IUPAC). Custom Defined Format uses the settings defined on the Setup Export tab.

If you select a folder that you do not have write permissions for, or if the location maps to an external drive or network location that is no longer available, after the scan has completed an error message will be displayed saying the data could not be saved. The spectrum will be added to a Samples View in the Data Explorer, so you can save the spectrum file or export the data to a different location.

If you enter a folder location that does not exist, but in a location you have write permission for, when the scan has completed the folder will be created and the file saved to that location.

If you have Spectrum ES you may be prompted for an electronic signature for the Data Export Collection signature point before the data is exported.

General - Show Live Display

By default, the Viewing Area displays your spectrum on the Live tab during scanning. Once the spectrum has been collected, the spectrum is displayed in the tab.

If you prefer not to see the Live tab, deselect this option.

Setup Instrument - Auto-Name

Use the Setup Instrument Auto-Name tab to set up a template for the Auto-name and Auto-description functions. These functions automatically enter names and descriptions for your samples.

1. Select **Instrument** from the Setup menu.

   OR

   Select  in the **Setup** section of the Navigation Pane.

   The Setup Instrument tabs are displayed in the Dialog Pane.

NOTE:	To see a the tabs, you may have to resize the Dialog Pane.

2. Select the Setup Instrument Auto-Name tab.

Auto-Name

Enter an auto-name format for your samples using a mixture of text and placeholders for variables. When you want to insert a placeholder, select the variable you need from the drop-down list.

The list of available variables enables you to include the date in several formats, your User Name or User ID, and to identify both the instrument and computer. You can also enter a Barcode.

The most important variable is Counter, placeholder [nnn]. This counter is incremented by 1 for each subsequent sample, which enables you to distinguish one sample from the next.

An example sample name enables you to check that your auto-name format is correct.

Auto Description

Enter an auto-description format for your sample using a mixture of text and placeholders for variables in the same manner as for an auto-name format.

An example description enables you to check that your auto-description format is correct.