Auszüge aus der MASsoft Anleitung

Diese Zusammenstellung sollen Ihnen helfen sich im Vorfeld mit der Software vertraut zu machen. Die Seitenzahlen sind nicht fortlaufend, folgen jedoch der Abfolge dieser Kurzanleitung. Da hier nur die grundlegendsten und für die Versuchsdurchführung nötigen Einstellung aufgeführt sind, fragen Sie im Zweifel Ihren Betreuer.

Auf den Seiten 3-9, und 2-7 lernen Sie die Hauptoberfläche mit der Menüleiste und der *Scan Gallery* kennen.
Auf Seite 10-7 werden die wichtigsten Knöpfe zum Betrieb des Quadrupol beschrieben. Sollten Sie längere Zeit keine Messung planen, dann schalten Sie die Emission aus (Knopf *shutdown*). Achten Sie auf den Steuerungskasten. Nur wenn dort die LEDs erloschen sind, ist das Gerät ausgeschaltet.

Die Seiten 4-4 – 4-10, 4-12 fassen die für Sie wichtigsten Scan Modi zusammen.
Von 7-21 bis 7-33 ist beschrieben, wie Sie die Ausgabe im grafische Messfenster verändern können (Achseneinteilung, Aussehen der Linie, . . .).

Die korrekte Auswertung der Umgebungsluftmessung erfordert ein Abzug des Untergrundes (Restgas). Die Subtraktion mittels dieser Software können Sie auf den Seiten 7-14 bis 7-18 nachlesen. Alternativ können Sie auch Ihre ins csv Format konvertierten Messdaten selbst bearbeiten.

Die Konvertierung in das csv Format sollten Sie für alle Messdaten durchführen. Anders können Sie später die Daten nicht verarbeiten. Das Speicherungsverfahren steht auf den Seiten 8-13 bis 8-15.

Für die Bearbeitung der Aufgabe A.6 müssen Sie die Linienbreite des Quadrupols ändern. Dies können Sie während einer laufenden Messung tun. Öffnen Sie das Menü *Tune→quad* und wählen dort die Option *delta-m%* aus. Geben Sie den gewünschten Wert im unkalibrierten Bereich von -100 – 100 ein. Beachten Sie, dass die Messung im aktuellen Zyklus durch das Tunen direkt beeinflusst wird. Sie können den Parameter auch bei angehaltenem Scan im *Global Environment Editor* ändern (Aufruf siehe nächster Abschnitt). Sie werden dann beim Starten der Messung (grüner Button) gefragt, in welcher Datei die Messung gespeichert werden soll (*New file*, *Append to current file* oder *Overwrite current file*).

In Aufgabe A.7 ist es zwingend erforderlich den Emissionsstrom zu reduzieren. Beachten Sie die Grafiken auf den Seiten 3-10 und 3-11. Deaktivieren Sie in der *Scan dialog box* (Seite 4-12) die Ckeckbox *Start scanning*. Nachdem Sie an alle nötigen Einstellung an dieser Stelle vorgenommen haben, öffnen sich die beiden Fenster *Scan tree* (S. 5-5) und *graphical view*. Doppelklicken Sie im *Scan tree window* auf die Box *Global: RGA*. Dies öffnet den *Global Environment Editor* (S. 6-14). Stellen Sie dort unter der Rubrik *Source* den Wert der Emission auf 60 μA ein. Klicken Sie auf OK und starten Sie Ihre Messung.

Wenn Sie für die Aufgabe A.10 als Detektor *total pressure* in der *Scan dialog box* einstellen, dann passieren Ionen aller Massen den Analysator und gelangen zum Detektor. Somit wird der Totaldruck im System ermittelt. Die Massenselektion (*start mass*, *stop mass*) ist irrelevant in dieser Einstellung. Sie spiegelt in diesem Fall jedoch eine Scanzykluslänge wider. Tragen Sie für einen langen Zyklus einen großen Massenbereich ein.

So ändern Sie bei angehaltenem Messzyklus den Detektionsbereich und ggf. die Zeitangaben *Dwell* und *Settle* (WICHTIG: die Daten im aktuellen Fenster gehen bei diesen Änderungen verloren.):
Öffnen Sie durch Doppelklicken im *Scan tree* (S. 5-5) die *Input Selection dialog box* mit der Beschriftung *Faraday* (S. 5-16). Sollten Sie bereits gemessen haben (ggf. Speichern) müssen Sie auf den Button *Unlock* klicken, um weitere Einstellungen vornehmen zu können. Sie werden darauf hingewiesen, dass nun alle aktuellen Daten verloren gehen. Ändern Sie nach belieben den Detektionsbereich. Die Zeiten *Dwell* und *Settle* können Sie entweder prozentual angeben oder direkt in Einheiten von Millisekunden. Die prozentualen Angaben beziehen sich dabei auf die werkseitig eingestellten Werte in Abhängigkeit vom gewählten Detektionsbereich und Scanmodus (S. 10-36).

3.3   Menu bar

The menu bar provides access to all MASsoft commands and contains the following menus:

File menu

Edit menu

MassSpecs menu

Tune menu

System menu

Views menu

Applications menu

Windows menu

Help menu

The menus are fully described in the Reference chapter of this manual, see Section 10.2.

3.4   Tool bars

The Tool bars contain buttons to provide quick access to common commands. The Tool bars, as shown in Figure 3.1, are displayed under the Menu bar and comprise four Tool bars arranged in one row, see Figure 3.2 below.
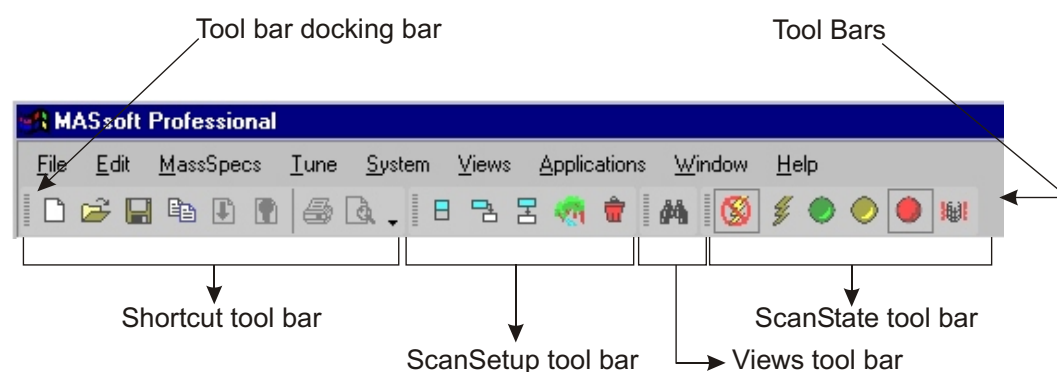

Figure 3.2 MASsoft Tool bars

Note

Some of the buttons may be grayed out if the command is not available.

The Tool bars may be hidden. To do this:

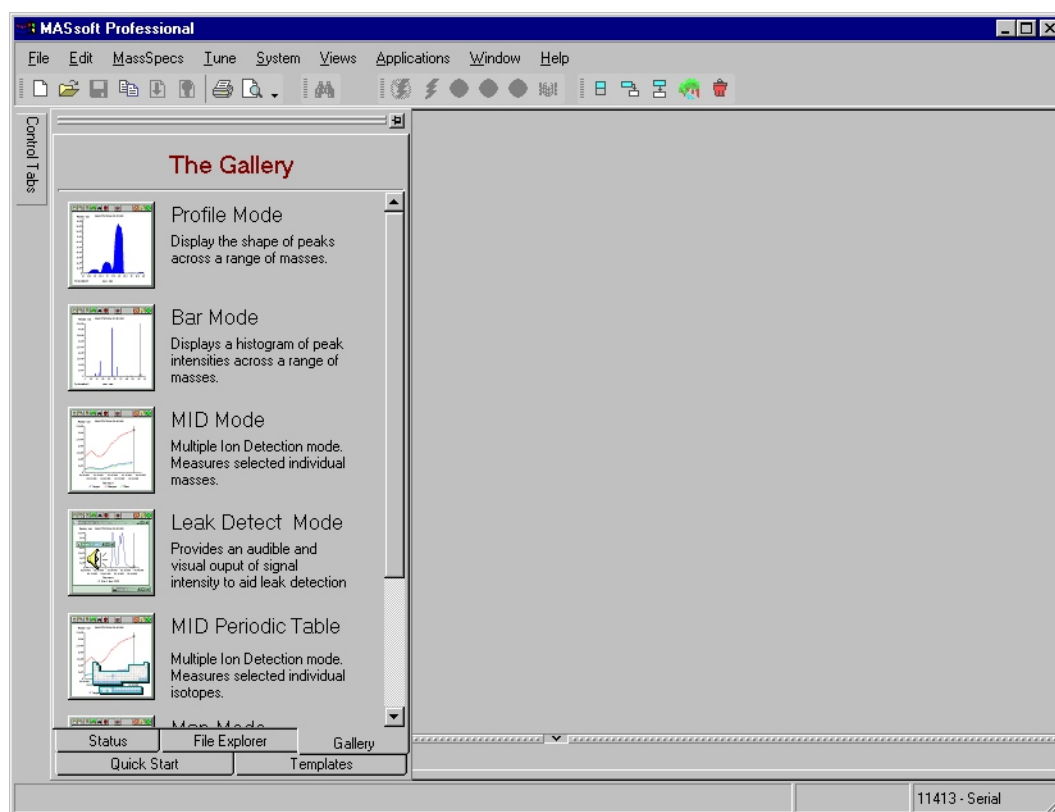|		
1.	Right click in the Tool bar.	The Tool bars menu, shown in Figure 3.3 will be displayed.
2.	In the Tool bars menu click the name of the Tool bar to be hidden.	Displayed Tool bars are marked with a tick.

Figure 2.3 MASsoft window

The MASsoft window is fully described in the Chapter 3 of this manual.

10.1.4   Scan State tool bar

	Shutdown	The Shutdown button stops data acquisition (if running), and puts the system into the Shutdown state by loading the values in the **Shutdown environment** box into the mass spectrometer. These would normally be set to remove any high voltages from the system e.g. the detector High Tension (HT) and 1st-dynode supplies and turn the ion source filaments either off or to a low value, but leave the system ready for operation at short notice.

The Shutdown button performs the same function as clicking **ShutdownAction** on the **System** menu.

	Power Up	The PowerUp button puts the mass spectrometer into a powered-up ('ready') state using the instrument mode information and variable values specified in the **Global** environment box at the top of the scan tree. If this is labelled **Global : RGA**, for example, the system is set to RGA mode.

This button does not start data acquisition.

The Power Up button performs the same function as clicking **Active** on the **System** menu.

	Start	The Start button (green) starts data acquisition; the mass spectrometer will be powered-up if it is in the shutdown state. If any changes have been made to the scan tree since the last acquisition or scan set-up operation, the new values are downloaded to the mass spectrometer before acquisition starts.

	Stop scan	The Stop button (amber) stops the scan at the end of the current cycle. When the end of the cycle is reached, this button is automatically deselected and the Abort button (red), is automatically selected.

	Abort scan	The **Abort** button (red) stops the scan as quickly as possible without waiting for the end of the cycle. If the **Shutdown after scanning** check-box in the **Stop** box **Scan structure cycles** dialog box is selected, selecting this button is equivalent to using the Shutdown button.

	Degas	The Degas button allows either filament to be switched on at a high electron energy for a certain time period; this heats the filaments and ion source cage which cleans them through forced degassing. Scanning cannot be performed whilst degassing.

The **Gallery** gives access to the following seven scan modes:

- Profile Mode
- Bar Mode
- MID Mode
- Leak Detect Mode
- MID Periodic Table
- Map Mode
- Surface Map Mode

When any of the above modes is started, by clicking the appropriate button, a scan dialog box will be displayed with variable values set to those last used.

4.1.1 Scan box items

Many of the dialog box items are common to a number of the scan modes, these items are described in this section. Unique dialog box items are described in the scan mode sections later in this chapter.

Mode	Sets the acquisition mode.
	This relates to the four operating modes; RGA, negative RGA, positive SIMS and negative SIMS not the scan modes. Depending on the instrument type and its options not all four operating modes may be available. For instance an RC RGA Analyser may only have the one RGA mode available.
Detector	Selects the detector (input device) to be used.
Acquisition range	Sets the acquisition range. The value entered directly is a power of ten; e.g. if **-7** is entered, the range set is 10^{-7}.
Auto range	When selected, the analyser automatically changes the range and follows changes in the input signal.
Linear	When selected, the display's Y-axis is linear.
Log	When selected, the display's Y-axis is logarithmic.
Log decades	Sets the number of decades on the log Y-axis.
	This is grayed out if **Linear** is selected.
View title	The title for the resulting view is entered in this box.
Start mass	Defines the scan start mass in amu.
Stop mass	Defines the scan stop mass in amu.
Auto scale Y-axis	When selected, the Y-axis is forced to fit the largest peak. When not selected, the Y-axis maximum will be set to suit the selected range.

Start scanning	If selected, scanning starts as soon as the **OK** button is clicked. If this option is not selected, the Tool Bar **Go** tool (green) can be used to start the scan.
Continuous scanning	Checking this box sets the instrument to scan continuously until it is stopped by the user.
Iterations	Selects the number of times the scan will repeat until it stops automatically. This is grayed out if **Continuous scanning** is enabled.

4.1.2   Profile Mode

Clicking the Profile Mode button in the Gallery opens the **Profile Mode** dialog box for a simple linear mass scan with **Start mass** and **Stop mass** variables, see Figure 4.2. It creates an analogue display on the automatically-attached view.
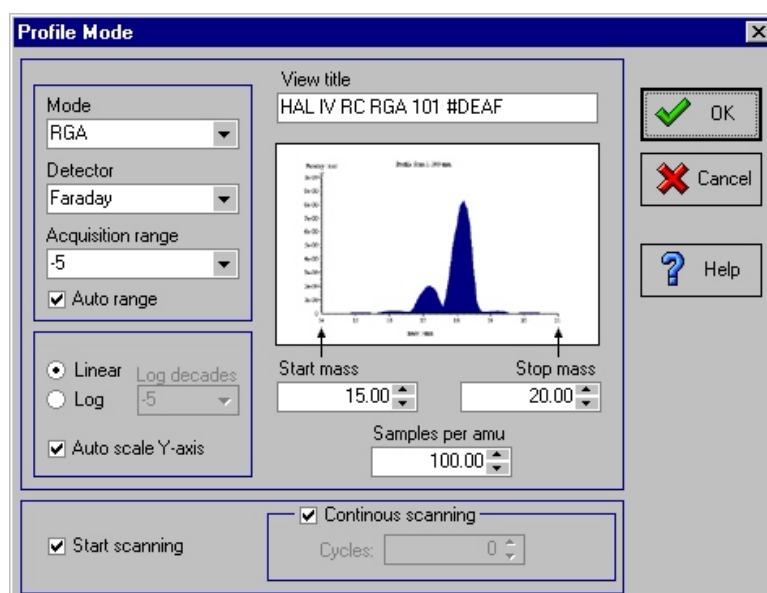
Figure 4.2 Profile Mode dialog box

Samples per amu	Sets the increment for the scan. This will determine at how many points across a 1 amu mass span the instrument will measure the partial pressure. For instance setting **Samples per amu** to 20 will result in 20 measurement points per amu (20 points per peak) a measurement every 0.05 amu.

The other dialog box items are common to other scan mode dialog boxes and are described in Section 4.1.1.

4.1.3 Bar Mode

Clicking the Bar Mode button in the Gallery opens the **Bar Mode** dialog box for a simple linear mass scan with a non-equal **Start mass** and **Stop mass**, and an increment of one amu, see Figure 4.3. It creates a histogram display on the automatically-attached view.
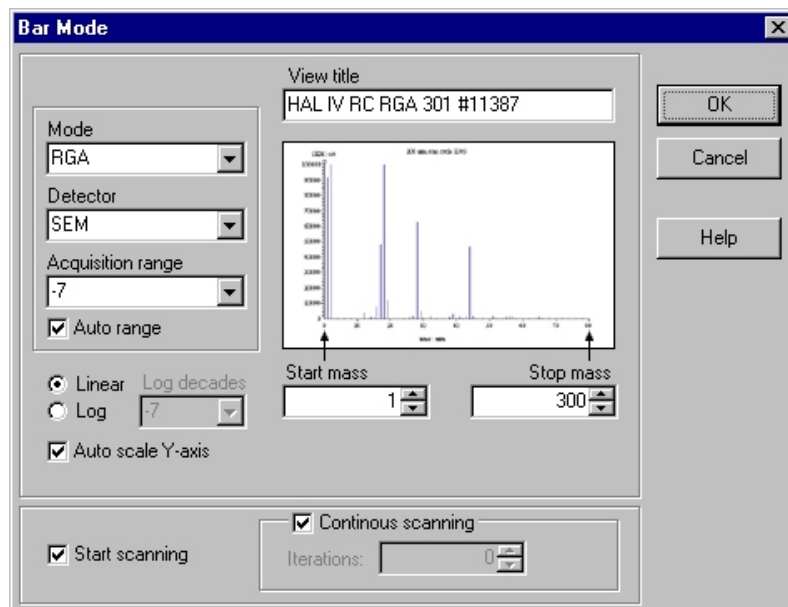

Figure 4.3 Bar Mode dialog box

All the dialog box items in the **Bar Mode** dialog box are common to other scan mode dialog boxes and are described in Section 4.1.1.

4.1.4   MID Mode

Clicking the MID (Multiple Ion Detection) Mode button in the Gallery opens the **MID Mode Scan** dialog box for multiple single mass scans with the option of building the scan tree by choosing from a **Library** list of components, see Figure 4.4. It creates a display for each monitored mass on the automatically-attached view.
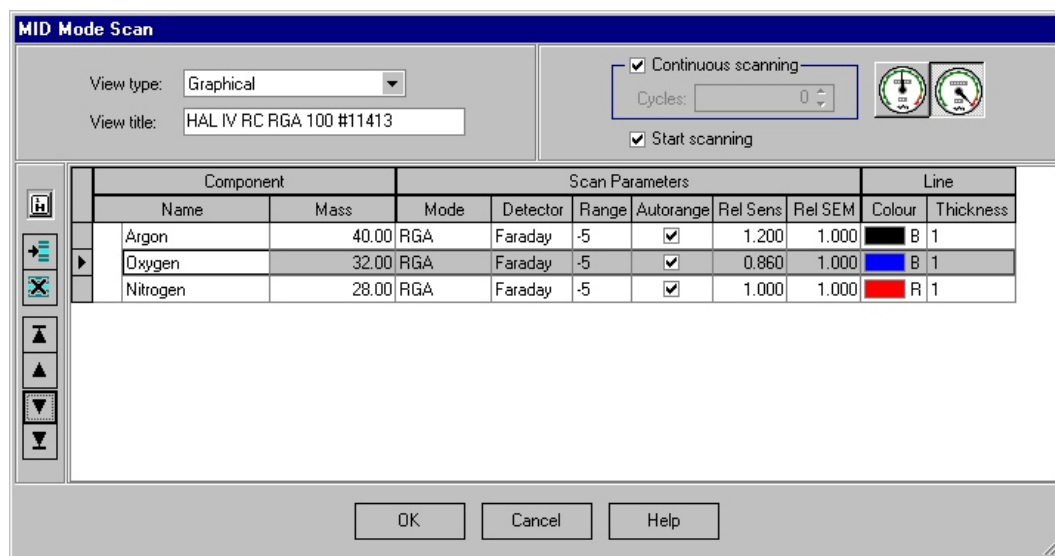
Figure 4.4 MID Mode Scan dialog box

Some of the dialog box items in the **MID Mode Scan** dialog box are common to other scan mode dialog boxes and are described in Section 4.1.1.

| **Optimise for Accuracy button**		The standard settings, 100% dwell and 100% settle, will be used.
Optimise for Speed button		Optimises the scan structure so that data can be acquired as quickly as possible; this is achieved by setting all scans in the scan tree to use the **Instrument mode** currently selected in the global **Environment Editor** dialog box. The **Dwell time** and **Settle time** are set to 3 ms and 2 ms respectively for scan structures containing a single scan; for scan structures containing multiple scans, the **Dwell time** and **Settle time** are set to 10%.
Add component from library button		Displays a drop-down list of components from the Library. Select the component to analyse. The major peak of the component will be added to the MID table, unless there is a conflict with another component in which case the **Alternative Peak Selection** dialog box is displayed.

Insert component button		Will add a new component after the currently selected component.
Delete component button		Deletes the selected entry from the components list.
To Top button		Moves the selected component to the top of the components list.
Move Up button		Moves the selected component up one place in the components list.
Move Down button		Moves the selected component up one place in the components list.
To Bottom button		Moves the selected component to the end of the components list.

To add a component from the library:

1. Select the component after which the new component should be added.

2. Click the **Insert Component** button.

3. Select the required library from the Library drop-down list box.

4. Select a component from the component list.

Possible conflicts due to overlaps in the cracking patterns of components are indicated in the **Component** name column by a yellow warning triangle .

Note

> *If two or more components have a common mass then a warning icon is displayed in the table's left hand column. Click on the warning icon to display details of the overlapping components.*

2. *If the chosen mass for a selected component has already been added to the table the Alternative Peak Selection dialog box is displayed from which an alternative can be selected.*
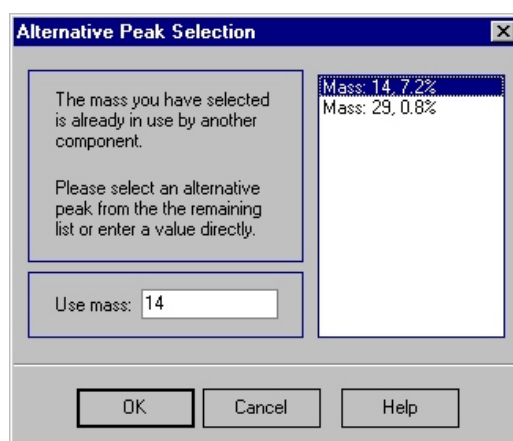
Figure 4.5 Alternative Peak Selection dialog box

To insert a new component:

1. Select the component after which the
    new component should be inserted.

2. Click the Insert component button.

3. Type the name of the new component
    into the Name field, and then press
    ENTER.

4. Enter the required values into the
    remaining fields.

To delete a component**:**

1. Select the component to be deleted.

2. Click the Delete component button.

Changing the order of the scans in a scan tree is a useful technique that can be used when
optimising an experiment for speed. In order to facilitate this there are a number of
controls on the MID, auto-tune and auto-mass align dialog boxes that can be used to
reorder the components in the table.

To move a component to the top of the table:

1. Select the component to be
    repositioned.

2. Click the To Top button.

To move a component up a place in the table:

1.   Select the component to be
     repositioned

2.   Click the Move Up button.

To move a component down a place in the table:

1.   Select the component to be
     repositioned

2.   Click the Move Down button.

To move a component to the bottom of the table:

1.   Select the component to be
     repositioned

2.   Click the To Bottom button.

4.1.6 MAP Mode

Clicking the **Map Mode** button opens the **Map Mode** dialog box for a simple linear scan with a choice of variable to be scanned and mass to be used, see Figure 4.7. It creates an analogue display on the automatically-attached view.

MAP scans are useful for selecting suitable variable operating points, for setting limits for auto-tune operations, or for appearance potential experiments where electron energy is scanned.
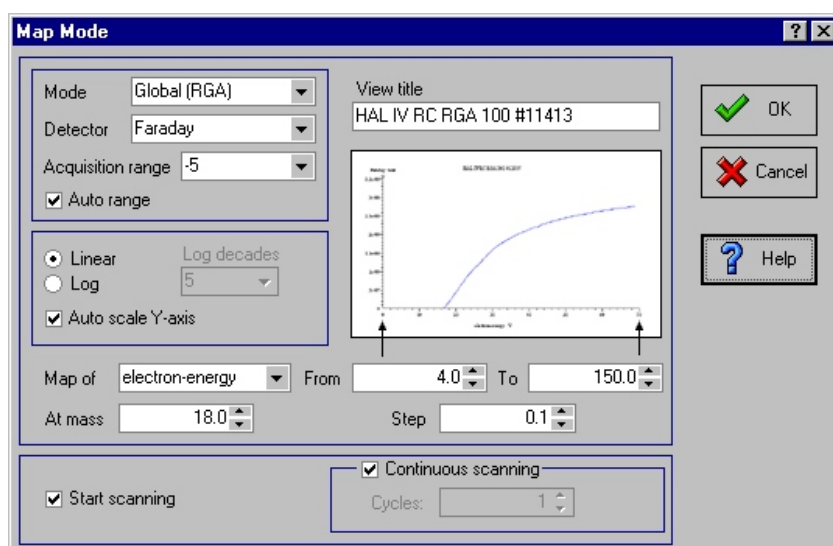

Figure 4.7 Map Mode dialog box

Some of the dialog box items in the **Map Mode** dialog box are common to other scan mode dialog boxes and are described in Section 4.1.1.

Map of	Sets the mapped variable. The variable name may also be typed directly in the box.

Note:

*The **Map of** list box only contains the commonly mapped variables; other variables can be entered by typing the name into the box.*

From	Sets the initial value of the variable specified in the **Map of** option.
To	Sets the final value of the variable specified in the **Map of** option.
At mass	Sets the mass at which the variable is to be mapped. The mass selected here is set into the **Global** box in the mass spectrometer control window.
Step	Sets the increment for the specified variable.

| 9. | Click the **OK** button. | The trends are added to the view. |

To remove trends from a graphical view:

1.	Select the view.	
2.	Click **Trend view setup** on the **Views** menu.	The **Trend view setup** dialog box is opened, see Figure 7.20.
		This dialog box is identical to that opened when creating a new trend view (see Figure 7.14), except that the **View type** list box is not present.
3.	Select the trend to be removed in the **Trends** box by clicking on it.	
4.	Click the **Remove** button.	The selected trend is removed from the **Trends** box.
5.	Steps 3 and 4 can be repeated for other scans in the **Trends** box, as required.	
6.	Click the **OK** button.	The trends are removed from the view.

7.4.4 Customising graphical views

Graphical views can be customised by pointing to **Properties** on the **Views** menu; this displays a sub-menu from which various commands can be selected, see Figure 7.21. This sub-menu can also be opened by right-clicking in the graphical view, but not within the graph itself.
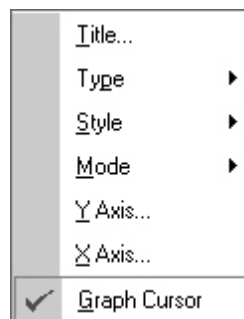

Figure 7.21 Views menu, Properties sub-menu

Title	Changes the view title.
Type	Changes the graph type (area, line or histogram).
Style	Changes the graph style (grid and axis value labelling).
Mode	Changes the graph mode (real time or historical data).
Y Axis	Changes the scaling of the Y-axis.
X Axis	Changes the scaling of the X-axis.
Graph Cursor	Turns the graph cursor on and off.

Changing the graphical view title

The title in the graph area of the view defaults to the name of the currently connected mass spectrometer.

To change this title:

1. On the **Views** menu point to **Properties** and click **Title** on the sub-menu.   The **Graph Title** dialog box is displayed, see Figure 7.22.

Figure 7.22 Graph title dialog box

2. Type the new title into the **Graph Title** box.   The new title does not change the Title bar of the window; this retains the name of the scan to which the view is attached.

3. Click the **OK** button.

Changing the graph type

To change the graph type of the selected view:

1. On the **Views** menu point to **Properties**   A sub-menu is displayed which lists the
    then point to **Type** on the sub-menu.   types of graph available, see
                                                   Figure 7.23.
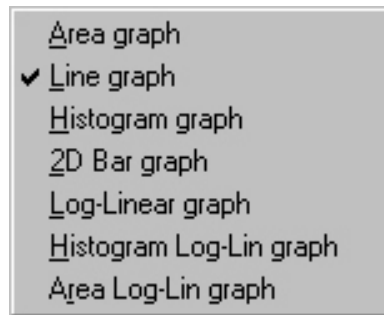
Figure 7.23 Views, Type sub-menu

2. Select the required option from the   The current data is displayed on a graph
    Views, Type sub-menu.   of the selected type.

                                             A tick indicates the currently selected
                                             type.

The options are:

Area graph   Fills in the area between the graph and the X-axis.

Line graph   Draws the graph as a line, with no fill between the line and
                          X-axis

Histogram graph   Each point on the graph is drawn as a histogram bar.

2D Bar graph   Each point on the graph is drawn as a two-dimensional
                          histogram bar.

Log-Linear graph   Draws the graph on a logarithmic Y-axis.

Histogram Log-Lin   As for **Log-Linear graph, but each point is drawn as a
graph**   histogram bar.

Area Log-Lin graph   As for **Log-Linear graph**, with the area between the graph and
                          the X-axis filled in.

Changing the graph style

1. On the **Views** menu point to **Properties** then point to **Style** on the sub-menu. A sub-menu is displayed which lists the available styles, see Figure 7.24.


Figure 7.24 Views, Style sub-menu

2. Select the required option from the **Views, Style** sub-menu. The style of the graph is changed to reflect the option chosen. Current styles are marked with a tick. As many style items as required may be selected.

The options are:

X Grid   Draws vertical lines over the graph at X-axis intervals.

Y Grid   Draws horizontal lines over the graph at Y-axis intervals.

7.4.4.1 Changing the graph mode

1. On the **Views** menu point to **Properties** then point to **Mode** on the sub-menu. A sub-menu is displayed which lists the available modes, see Figure 7.25.

Figure 7.25 Views, Mode sub-menu

2. Select the required option from the **Views, Mode** sub-menu. Where a view is attached to a scan acquiring data, the normal display would show the latest data as it is acquired, i.e. **Real time**.

The options are:

Real time   Displays the latest cycle, or, in the case of trend data, the last few cycles acquired. If viewing data from a data file, cycle number 1 will be displayed; select **Historical data** to view other cycles.

Historical data   This is used to look at data already acquired; a scroll bar is added to the view which allows the time scale of the X-axis to be scrolled backwards and forwards, see Figure 7.26. The scroll bar can be used to move through the data, alternatively, a specific cycle number can be typed in the **Cycle number** text box.

Note:

The **Historical data** *command only applies to* **Bar** *and* **Profile** *type views; an alternative method (for* **MID** *trend views only) is to use the click and drag zoom facility to extend the viewed region.*
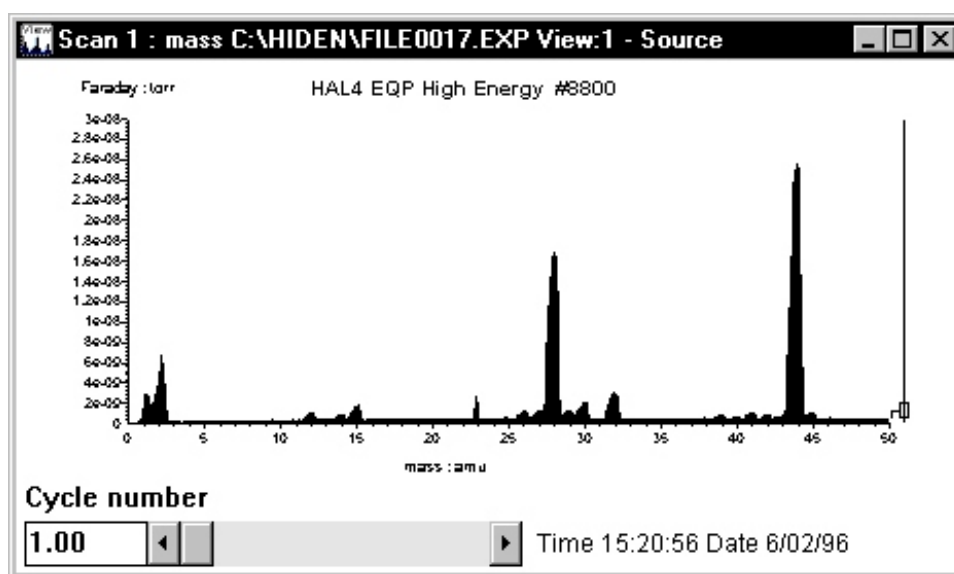

Figure 7.26 View with Historical data scroll bar

7.4.5   Scaling a Y-axis

The display and scaling of a Y-axis can be altered either by double-clicking on the Y-axis to be scaled, or by selecting **Views**, **Graphical, Y axis** (in the case of a graphical view having two Y-axes, the Y-axis to be scaled must be selected before selecting the **Views**, **Graphical, Y axis;** a small arrowhead will appear above the selected axis). In either case the **Y Axis Properties** dialog box is opened, see Figures 7.27 and 7.28.
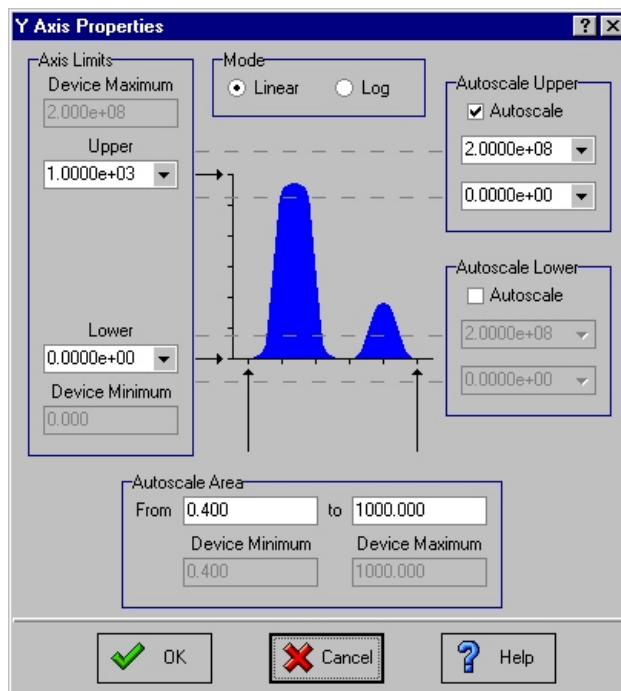
Figure 7.27 Y axis properties dialog box

The **Axis limits** frame contains the following controls:

Upper   This combination box sets the Y-axis upper limit. The value
                     may also be entered directly into the box. This value defaults to
                     the maximum value on the start range of the scan's input device
                     or 1000 counts per second for pulse counting systems.

Lower   This combination box sets the Y-axis lower limit; the value may
                     also be entered directly into the box; this value defaults to **0.0**.

Note:

Positive or negative values can be entered in the **Upper** *and* **Lower** *combination boxes.*

Linear   When selected, the display's Y-axis is linear.

Log   When selected, the display's Y-axis is logarithmic.

Note:

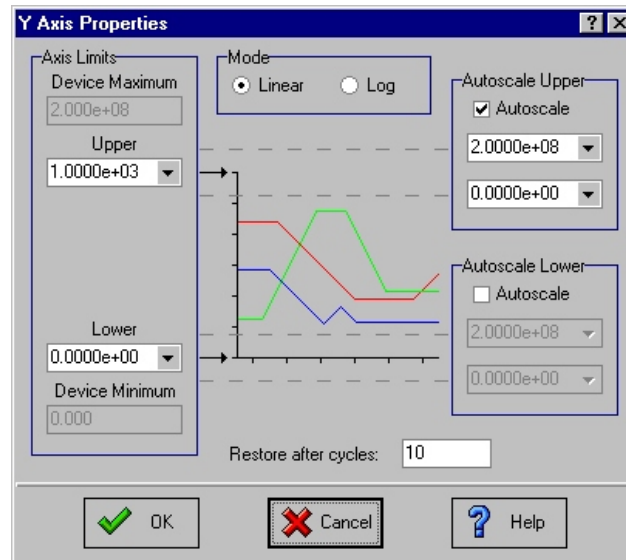*Either* **Linear** *or* **Log** *can be selected, but not both.*

Figure 7.28 Y Axis Properties, MID views

Autoscale upper	Checking this option turns on the Y-axis upper limit autoscaling.
	The option is accompanied by two combination boxes which specify the upper and lower values between which the autoscale algorithm may set the Y-axis upper limit. The limits may also be entered directly into the boxes.
Autoscale lower	Checking this option turns on the Y-axis lower limit autoscaling.
	The option is accompanied by two combination boxes which specify the upper and lower values between which the autoscale algorithm may set the Y-axis lower limit. The limits may also be entered directly into the boxes.
Autoscale area from … to …	These text boxes specify the X-axis boundaries between which the Y-axis autoscaling data is taken; this can be used to prevent a large peak swamping lower-level data by setting the boundaries such that data from the large peak is excluded.
	This function will not appear in the **Y axis attributes** dialog box if the selected view is a **MID** trend view.

Restore after cycles	This value indicates the number of cycles displayed before the system checks for under-range on the Y-axis (e.g. if the intensity of the displayed data drops for a number of cycles before rising again, the Y-axis upper limit is not immediately adjusted to a lower value over this number of cycles).

7.4.6   Scaling the X-axis

The display and scaling of the X-axis can be altered either by double-clicking on the X-axis or by selecting **Views**, **Properties, X-axis....** In either case the **X Axis Properties** dialog box is opened, see Figure 7.29 and 7.30, which provide control of the X-axis.
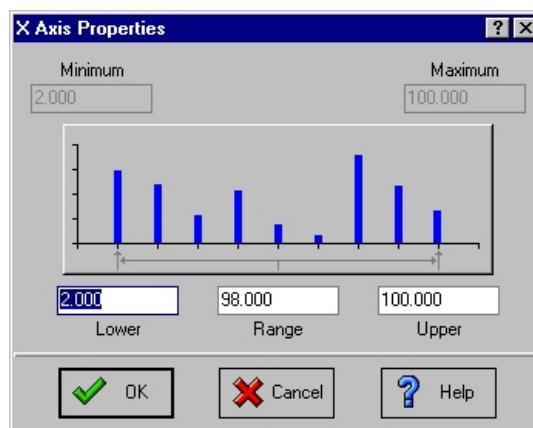

Figure 7.29 X Axis Properties dialog box

X minimum	Displays the minimum value of available X-axis data.
X maximum	Displays the maximum value of available X-axis data.
Lower	The X-axis lower limit can be entered directly in the box.
Range	The range between the X-axis **Upper** and **Lower** limits can be entered directly into the box.
Upper	The X-axis upper limit can be entered directly in the box.

Note:

1. *If the* **Upper** *value is set, the* **Range** *value will be altered to be the difference between the* **Upper** *and* **Lower** *values.*

2. *If the* **Range** *value is set, the* **Upper** *value will be altered to be the* **Lower** *value plus the* **Range** *value.*
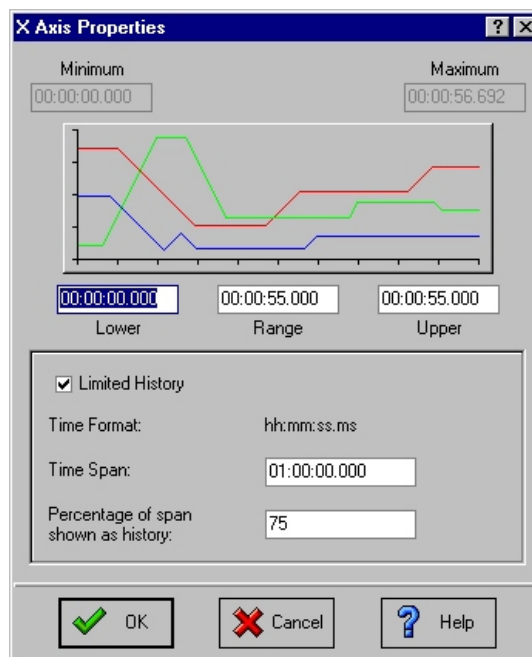
Figure 7.30 X Axis Properties, MID views

Limited history	When selected, the amount of data on the screen is limited to the time range shown in the **Time span** box.
	If this box is not checked and the display is zoomed out, the display extends from the start of the acquisition to the present time; for long acquisitions this may lead to a loss of display resolution.

Note:

If **Limited history** *is not selected, MASsoft will eventually run slowly in long acquisitions due to the large amount of data that has to be redrawn. This can be avoided by selecting* **Limited history***, in conjunction with a short* **Time span***, or by using a tabular view rather than a graphical view.*

Time span	The time range can be entered in this text box when the **Limited history box** is checked.
% of span shown as history	When the data reaches the right-hand edge of the display, the display has to be redrawn to make room for more data. The **% of span shown as history** value defines the amount of data that is retained and shifted to the left of the display.

Note:

Limited history, History period *and* **% of span shown as history** *only appear in the* **X Axis Properties** *dialog box when the graph is a MID or trend display.*

Graph cursor

The graphics cursor is displayed during acquisition when the **Views**, **Properties**, **Graph cursor** is ticked.

To turn off the cursor, click **Views**, **Properties**, **Graph cursor** to remove the tick.

7.5 Mouse operations

Click and drag zooming

In any graphical view window, the displayed axis limits may be set interactively using the mouse in addition to being able to edit the X- and Y-axis values in the associated dialog box.

a) Expanding a view in two dimensions

Data may be "zoomed" in two dimensions by using a "rubber band" box:

1. Move the mouse pointer to one corner of the area to be zoomed and hold down the left mouse button.

2. Move the mouse to draw out a rectangular box the corner of which follows the pointer.

3. Release the mouse button.   The area within the box is expanded to the full size of the window.

Figure 7.31 shows the result of expanding the X- and Y-axes in line with the action shown in Figure 7.32.
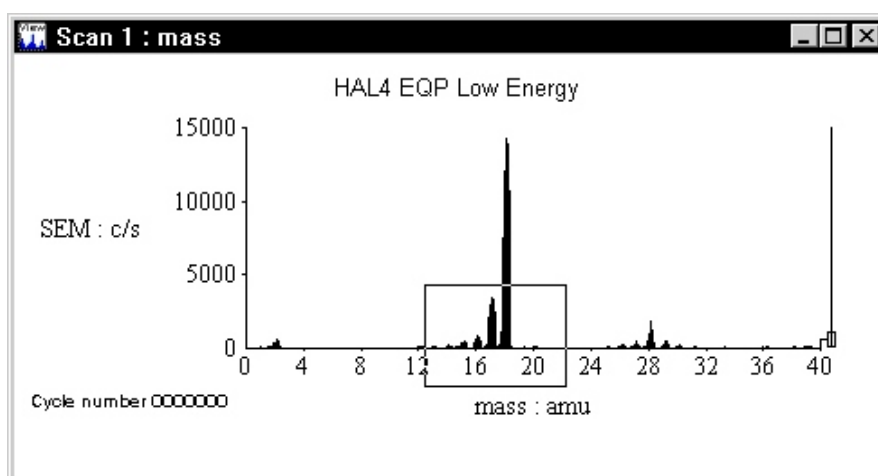

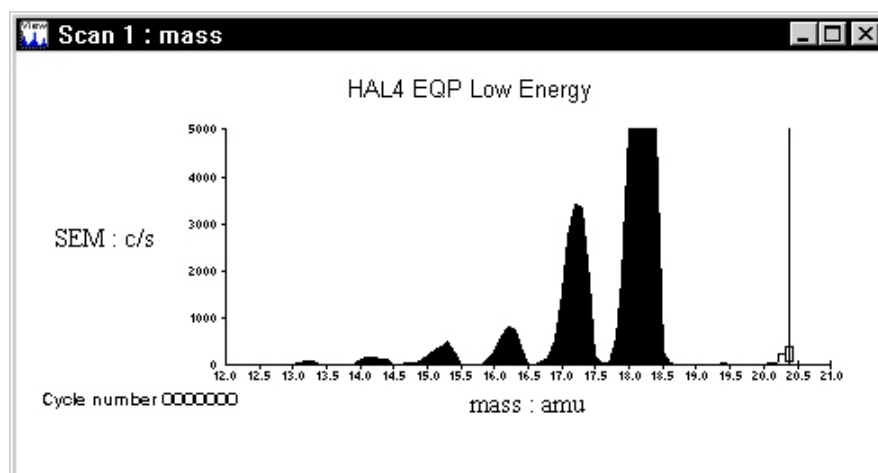**Figure 7.31 Two-dimensional expanded view 1**

Figure 7.32 Two-dimensional expanded view 2

b) Expanding a view in one dimension

1. Hold down the left mouse button and move the mouse pointer only vertically or horizontally.

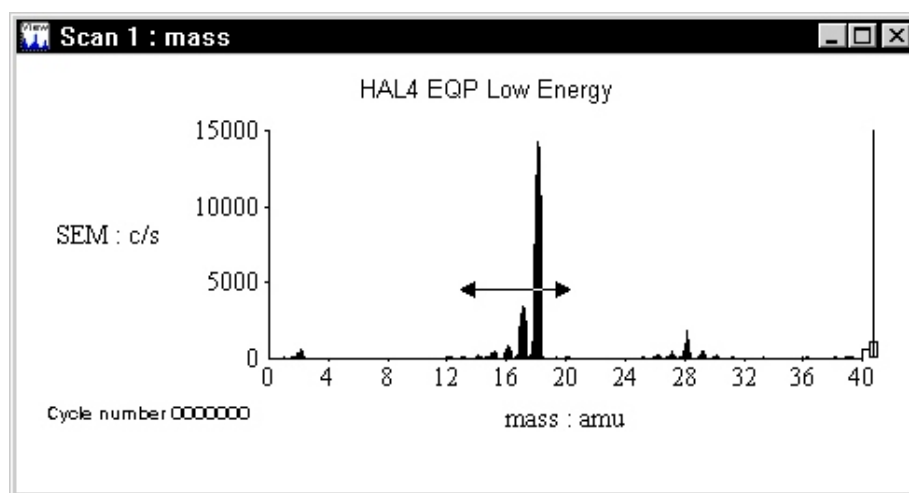   An arrowed line is drawn out, see Figure 7.33.

Figure 7.33 One-dimensional expanded view

2. Release the mouse button.

    The axis parallel to the arrow is expanded to match the size of the arrow, but the other axis is unchanged.

c) Restoring a view

After a view has been zoomed, it can be restored to full scale by similar techniques, see Figures 7.34 and 7.35. If the dragged rectangular box, or arrow, starts and/or finishes outside either of the current axis limits, those axes are restored to their maximum limits.
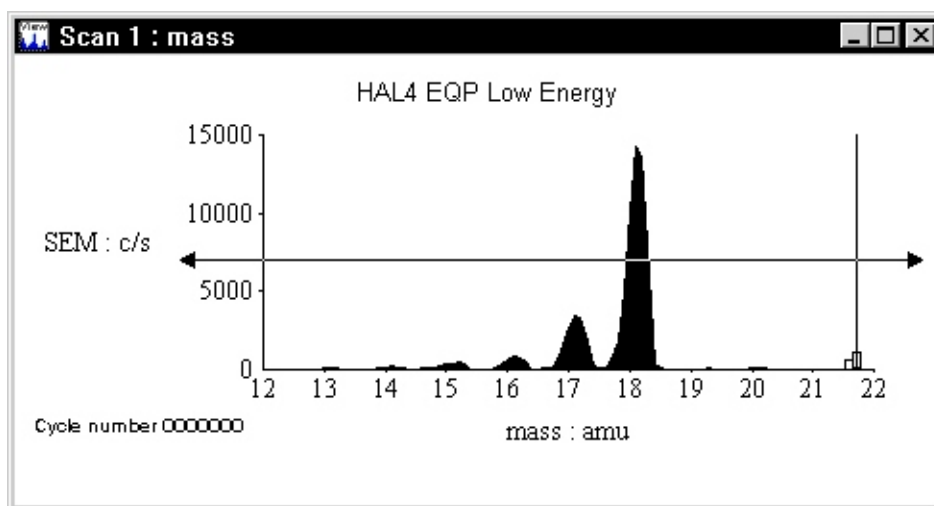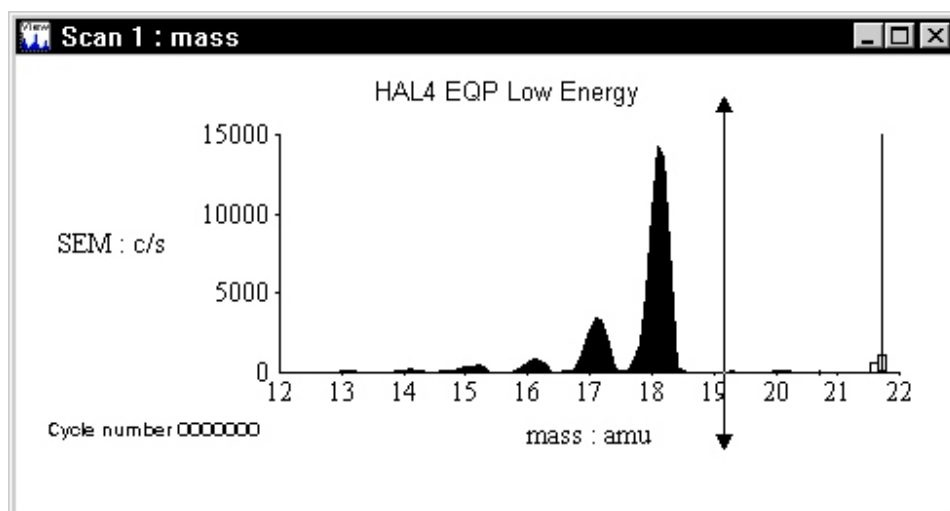

Figure 7.34 View marked for X-axis restoration

Figure 7.35 View marked for Y-axis restoration

Line Colour	The line colour for the resulting trend display can be selected in this list box. **Line colour** will scroll through the available colours as further scans are selected from the **Available scans** list.
Line Width	The line width for the resulting trend display can be selected in this list box; the higher the number, the thicker the line. **Line Width** defaults to **2**.
Add	Adds the selected scan and trend details to the top of the list in the **Trends** box.
Remove	Removes a selected trend from the **Trends** box.
Trends	This box contains the list of trends derived from the **Available scans** list and **Trend value** box. Trends are added to the top of the list by clicking the **Add** button. A selected trend is removed from the list by clicking the **Remove** button.
View type list box	Selects the type of trend view that is produced when the **OK** button is clicked. The options are:
Graphical	Produces a graphical trend view; this is the default **View type** option.
Tabular	Produces a table of the trend view data.
One of each	Produces a graphical trend view and a table of the trend view data.

7.3.2   Background subtract

The Menu Bar **Views**, **Background subtract** function subtracts the data values in one view (the "source" view) from the data values in a selected "target view", with the result being displayed in the "target" view. An operations window, describing the operation that has been performed, is displayed by default in the target view.

Background subtract works on both graphical and tabular views; the views can be from different data files.

Note:

It may be found useful to tile the views (using the Menu Bar **Window***,* **Tile vertical** *or* **Window***,* **Tile horizontal** *command) before using* **Background subtract***.*

To use **Background subtract**:

1.   Select the view which contains the data values that are to be subtracted from the data values in the "target" view.

2. Click **Source view** on the **Views** menu.

The selected view becomes the "source" view, see Figure 7.15 or an example graphical view.

If the "source" consists of graphical MID data, the **MID Data source** dialog box will appear, see Figure 7.16.

This prompts the user to enter the cycle containing the data which is to be subtracted, as a constant, from the "target" data. Select the required cycle and click the **OK** button before continuing.

If the "source" is a tabular view, the MID Tabular data source dialog box is opened, see Figure 7.17. This dialog box allows the user to select the cycle or statistical data to be subtracted from the "target" data.
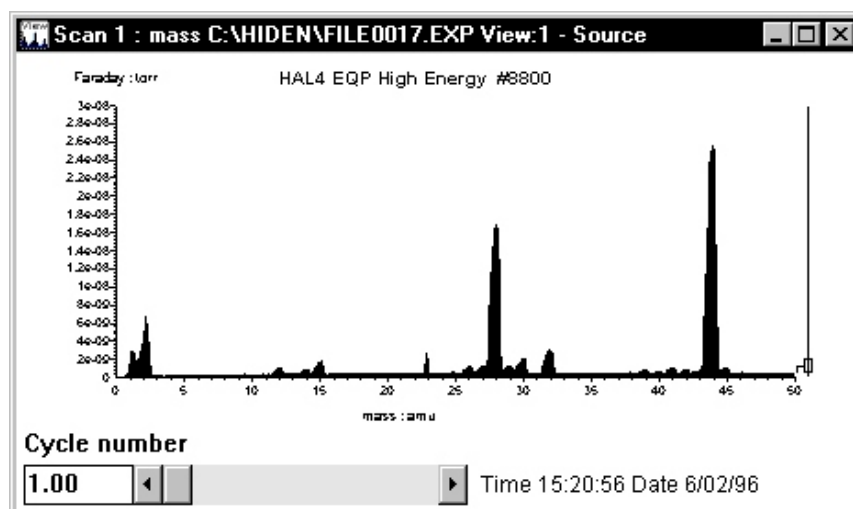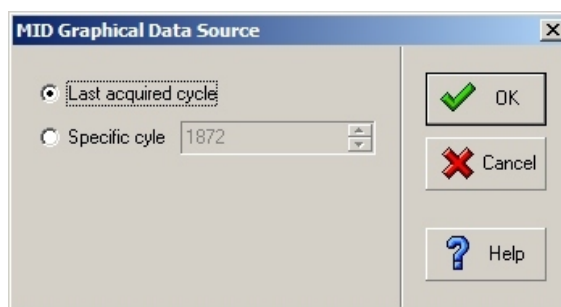

Figure 7.15 Example "source" view
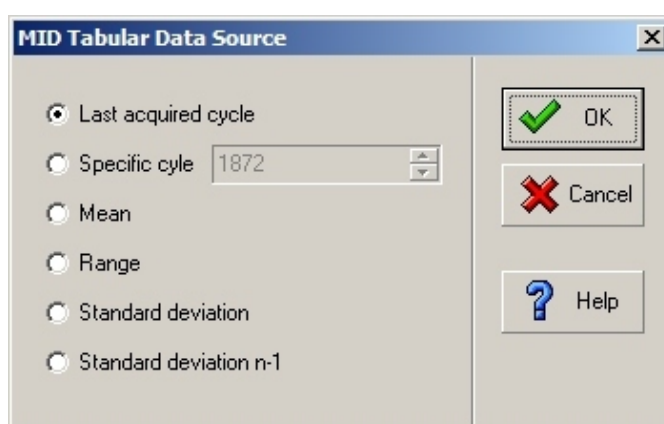
Figure 7.16 MID data source dialog box

Figure 7.17 MID Tabular data source dialog box

3. Select the view which is to be the "target" view.

    See Figure 7.18 for an example "target" view.

4. Click **Background subtract** on the **Views** menu.

    The "source" data is subtracted from the "target" data and the result displayed in the "target result" view, see Figure 7.19.

    An operations window is displayed, by default, in the "target result" view; it gives brief details of the **Background subtract** operation(s) used to create the view.

Note:

It is possible to subtract several different "sources" from one "target", hence the operations window can contain more than one operation.
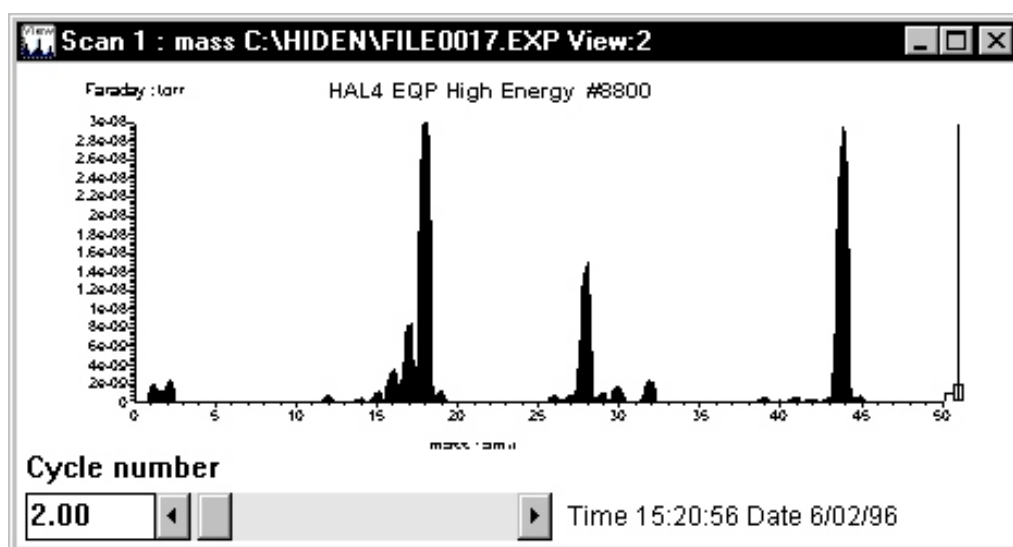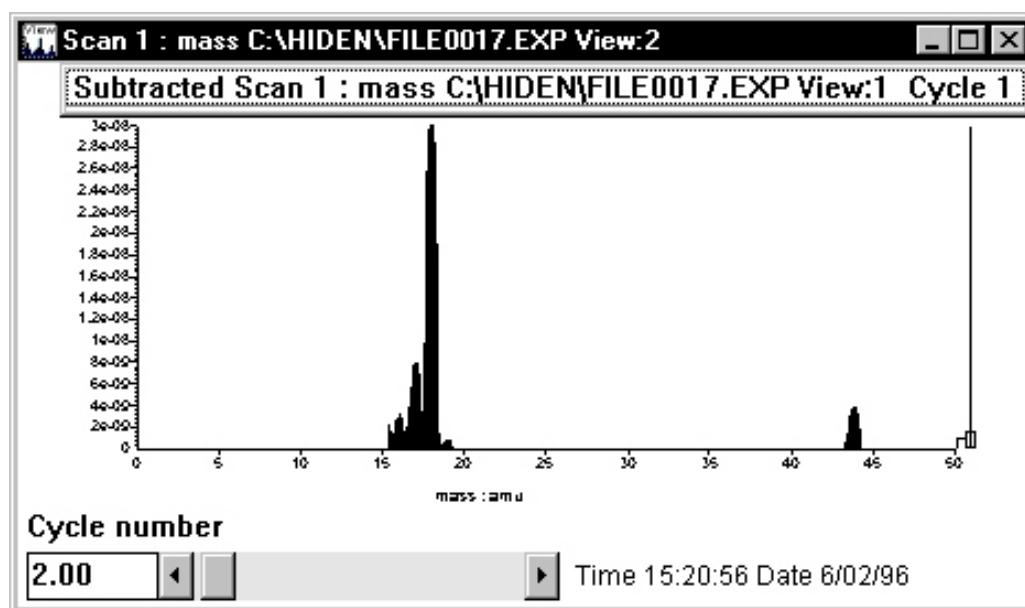
Figure 7.18 Example "target" view

Figure 7.19 "Target result" view

5. If required, the operations window can be turned off by clicking **S**how **operations** on the **Views** menu.

The operations window can be switched back on by clicking **Show operations**, on the **Views** menu again.

6. A "source" view can be deleted from the operations list by clicking on it and then clicking the **Delete** button

 .

7.4 Graphical views

A graphical view displays data in the form of a graph; the view can be customised to suit the user's requirements.

The **New graph view** command on the **Views** menu, or the Attach view button , are used to add a graphical view to a selected scan. MASsoft will try to create the right type of view based on the values in the scan. The examples in Section 7.2 should make this clear.

Trend views are created by clicking **Trend view setup** on the **Views** menu. Scans created from the **Scan Gallery** have views attached automatically and may have additional views attached, e.g. to zoom in on an area of interest or to simultaneously review data whilst displaying live data.

Data recorded in files may be viewed using the menu bar **Views, Graphical**, **Mode**, **Historical data** command.

7.4.1 Creating a graphical view

To create a new view, either:

1. Select a scan in the scan tree.

2. Click **New graph view** on the **Views** menu.

   A new view window is created and the data in the scan are drawn in it.

or:

1. Select a scan in the scan tree.

2. Click the Attach view, button.

   A new view window is created and the data in the scan are drawn in it.

The data cycle displayed in the view can be selected by using the **Views**, **Graphical**, **Mode**, **Historical data** command.

8.4 Exporting data

Data may be exported in various formats for use in other applications.

8.4.1 Windows screen copy

A bitmap copy of all or part of the MASsoft application screen can be made using the normal Windows copy options. To copy an active MASsoft application window, press the *Alt*, *Print Screen* key combination. To copy the whole screen, where MASsoft is not maximised, press the **Print Screen** key. With either method, the resultant bitmap may be copied into other Windows applications by pasting from the clipboard.

8.4.2 Exporting ASCII and DDE data, and copying to the clipboard

Data may be exported for use in other graphics packages and spreadsheets by clicking **Export** on the **File** menu which provides two export options:

- **File** enables the current data to be exported as an ASCII file for use by other packages.

- **DDE** provides the ability to transfer, in real time, data to other Dynamic Data Exchange (DDE) client-compatible applications by defining the relevant data and then using **Edit, Copy** to copy the data to the clipboard.

ASCII file format

When **File**, **Export**, **File** is selected, the **Export Information** dialog box is opened, which requests an output file name, see Figure 8.10.

When a name has been entered in the **File Name** box, clicking the **OK** button produces a file of ASCII values separated by the default Windows separator character for the view currently selected. For a normal sequence or co-variant scan, the whole of the scan is exported, but when a multi-variant scan is selected, the whole of the major (i.e. highest level) scan is output, which may include several subordinate scans, resulting in a large output file. The **.csv** extension name allows the resultant file to be read into other applications as ASCII comma-separated values, after which the data can be manipulated as required.

Refer to the Windows Control Panel documentation for details of the Separator character and International settings.

Note

In Windows XP the separator character can be checked/edited by:

*Double clicking **Regional and Language Options** on the **Control Panel**, selecting the **Regional Options** tab, clicking the **Customize...** button which opens the **Regional Options** dialog box. The **List separator:** value box on the **Numbers** tabs defines the separator character.*

CAUTION

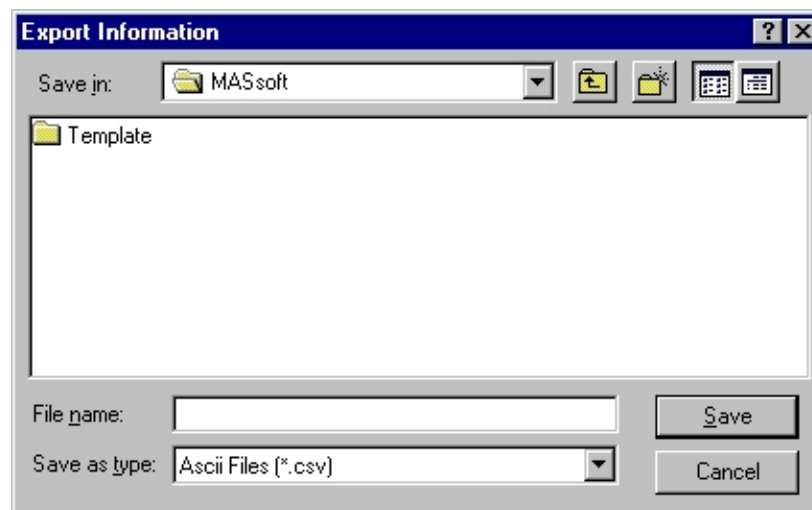**Changing the Separator character may cause MASsoft and other Windows applications to function incorrectly.**

Figure 8.10 Export Information dialog box

DDE and copying to the clipboard

Selecting **Export**, **DDE** on the **File** menu opens the **DDE link selection** dialog box, see Figure 8.11.
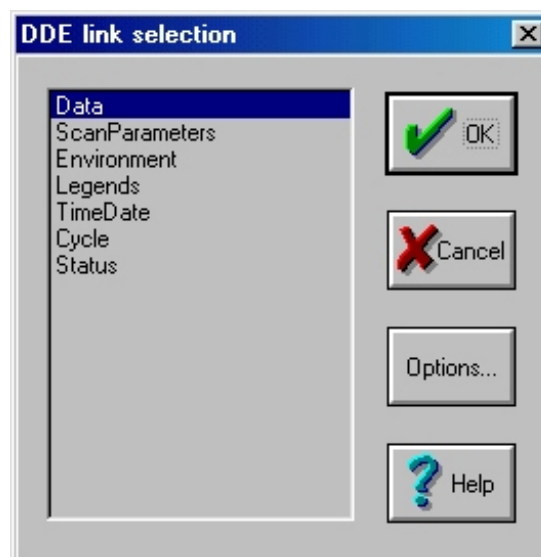

Figure 8.11 DDE link selection dialog box

The type of information to be linked is selected by clicking on it, then clicking the **OK** button. To transfer information, select the view containing the scan to be copied or linked, click **Copy** on the **Edit** menu to transfer the information to the clipboard. The

client application can then import the data using the **Edit**, **Paste** command, or link to it, using the **Edit**, **Paste Special** command.

Note:

*When a view is copied to the clipboard, using the **Edit**, **Copy** command, two sets of data are transferred. One set is text data, which allows DDE values to be transferred, the other is the view as a Windows metafile picture. If the **Edit**, **Paste** command is used when pasting the data into another application, the client application will take the most suitable data set for its normal operation. For example, a word processor will take the text, whereas a drawing application will take the picture.*

*To force the client application to take the other data set (for example, a picture into a word processor) the **Edit**, **Paste Special** command must be used; this allows the input object to be selected. If the **Paste:** option in the **Paste Special** dialog box is selected, the data is copied into the client application and the transfer ends. If the **Paste Link:** option in the **Paste Special** dialog box is selected, a link is set up between the client and the MASsoft server. If the data in the MASsoft view now changes (e.g. during acquisition) the new data will automatically be transferred to the client. This "hot link" can be used with a spreadsheet, for example, to extend MASsoft's data-processing capabilities.*

The **Options...** button is only available if the selected information is **Data** and the view is a Multiple Ion Detection (MID**)**-type. Selecting this button opens the **MID data** dialog box, which allows the **Number of cycles** and **Time Formats** to be selected, see Figure 8.12 each individual time format, or both time formats, can be selected.
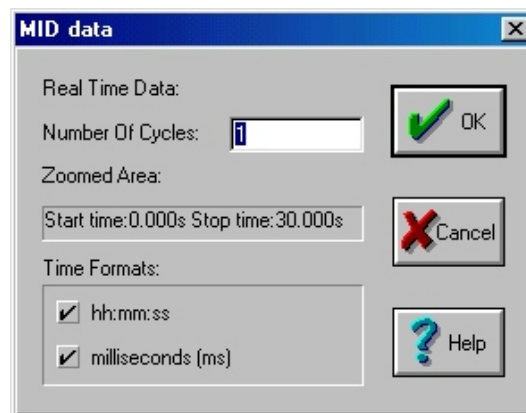

Figure 8.12 MID data dialog box

3.6 Filament operation at reduced electron energy

[hand icon]	**CAUTION** **Using too high an emission value may damage the filament.**

electron energy can be set to a minimum value of 6 eV. When **electron energy** is to be scanned from less than 20 eV, the emission current must be reduced in order to protect the filaments from damage due to excessive current demands.

Figures 3.2, 3.3 and 3.4 should be used as guides for safe operation of the filaments at reduced electron energies. Referring to Figure 3.2, for example, for an emission current of 400 A, the demanded filament current changes slowly with decreasing electron energy until the electron energy is approximately 18 eV. A rapid increase in demanded filament current then occurs due to changes in the emission characteristics. Running the filaments in this region may lead to filament damage. The onset of this region occurs at lower electron energy values as the emission current is decreased.
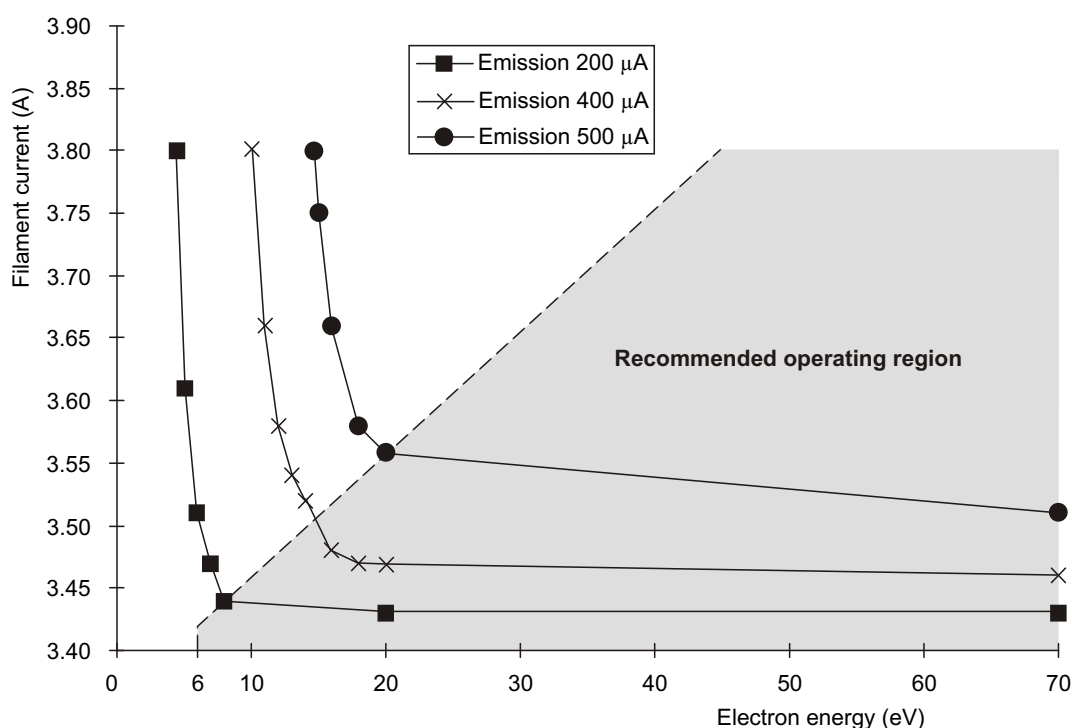

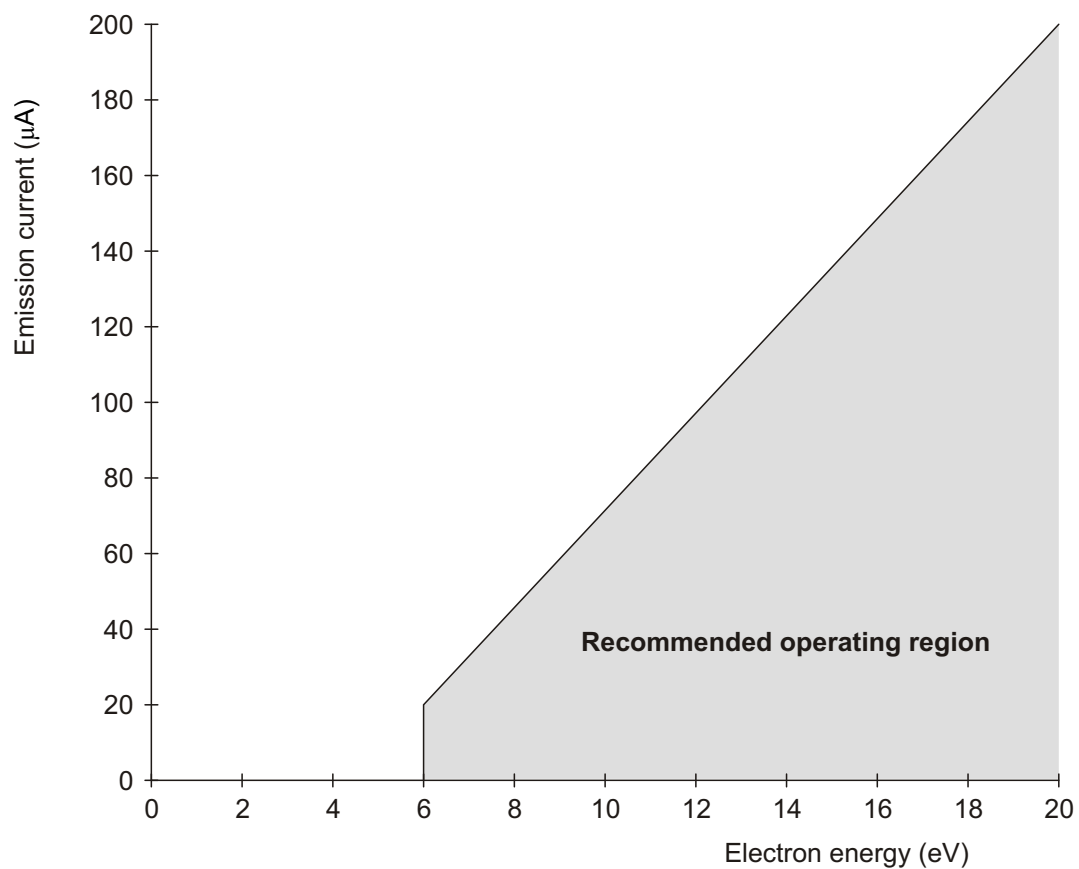**Figure 3.2 Variation in filament current with electron energy**

Figure 3.3 Emission current - minimum electron energy characteristic: 0 to 20 eV
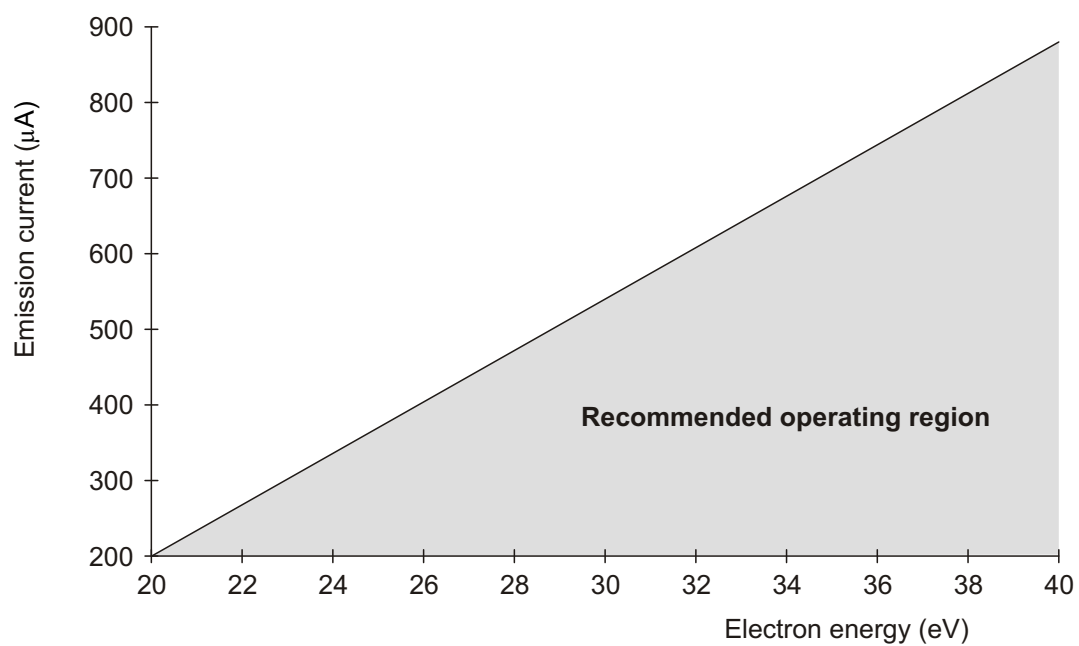

Figure 3.4 Emission current - minimum electron energy characteristic: 20 to 40 eV

5.1   Scan tree window

The **MASsoft** window holds the scan tree window (or windows: several scan tree windows, for different instruments, or for the same instrument, may be open at the same time), see Figure 5.1.
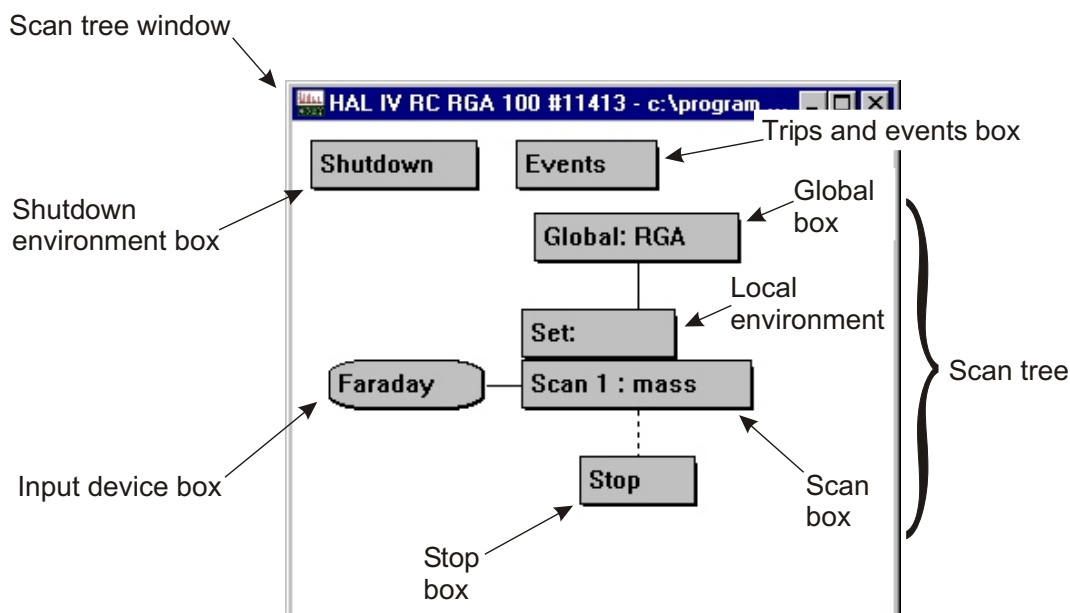

Figure 5.1 Scan tree window

The scan tree window title bar contains the name of the instrument and its access status (i.e. "Available" or "Unavailable"). Each scan tree window contains a description of the way the instrument behaves when asked to acquire data, in the form of a graphical diagram, or scan tree, see Section 5.2. The total description held in the window is called an "experiment"; it comprises a series of environment, scan and scan control boxes. This description may be modified by adding extra environments and scans, and by altering their variable values. The contents of the scan control boxes in the scan tree window can be edited by double-clicking on them.

The scan is the heart of the mass spectrometer controller; the Hiden Analytical Limited scan generators have been designed to be powerful and as flexible as possible.

A scan can be one of three types:

1. A simple scan, where a single variable is scanned by incrementing between defined start and stop values, see Section 5.5.1.

2. A co-variant scan, where two or more scans are linked so that each updates its output before another data point is acquired; it is used to allow variables to track one another, see Section 5.5.2.

3. A multi-variant scan, where two or more scans are linked so that subordinate scans perform a complete scan before the next higher scan in the tree updates its output.

6.4 Global environments

The global environment encompasses the variable values of all the acquisition modes. The global environment for each acquisition mode contains the current device values for that mode. These device values are used whenever that acquisition mode is selected for a scan, unless overridden by a local environment associated with that particular scan.

The device values for each type of acquisition mode can be edited using the **Global Environment Editor**, see Section 6.4.1 for information on managing the global environment device values. The acquisition mode of all the scans using the global mode can be changed by selecting the required mode in the **Global Environment Editor** dialog box.

The Global Environment is stored in the Experiment file.

6.4.1 Scan Global Environment Editor

The **Global** box holds the global environment values for all modes and defines which acquisition mode is used when the global mode is selected in the scan. The environment values may be edited by double-clicking on the **Global** box, which opens the global **Environment Editor** dialog box, see Figure 6.4.
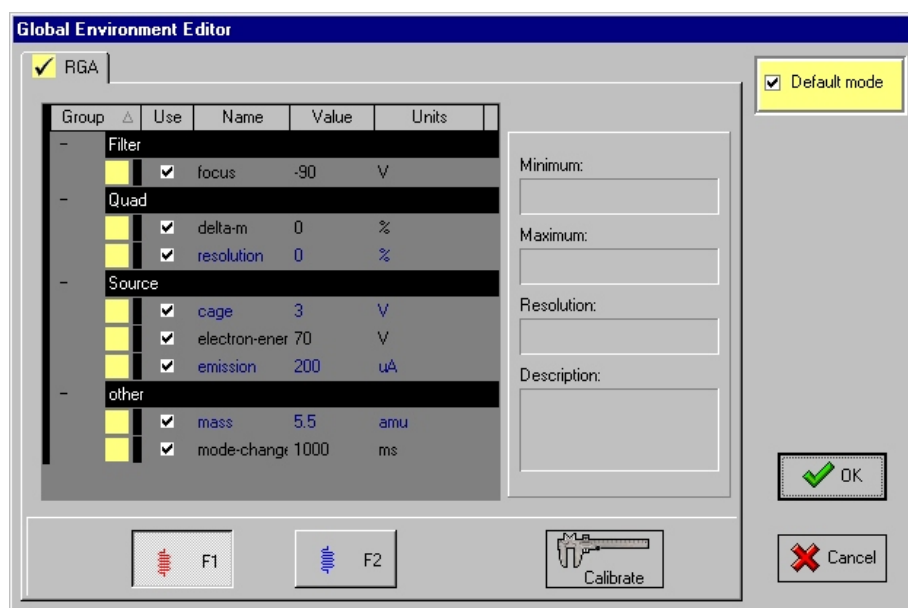

Figure 6.4 Global Environment Editor dialog box

5.4 Input Selection dialog box

Double-clicking the **Input device** box (see Figure 5.1 and Section 5.1) opens the **Input Selection** dialog box, see Figure 5.6. If the mass spectrometer supports more than one input device, the **Input Selection** dialog box allows selection of the input device used by a scan.
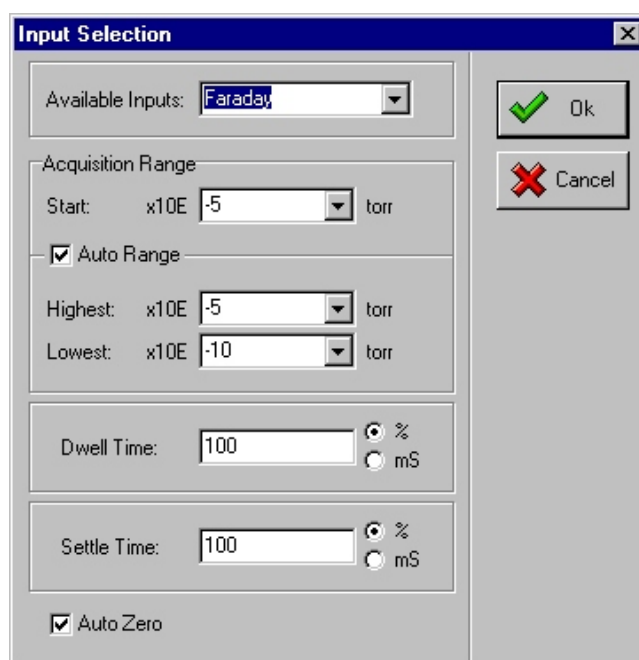
Figure 5.6 Input Selection dialog box

The dialog box supports range-switched input devices and allows the user to specify upper and lower auto-range limits to prevent auto-ranging to slower, high-gain ranges when very small peaks are not of interest, or to low-gain ranges which would suppress very small peaks.

Available inputs   The **Available inputs:** combination box contains a list of the input devices available on the instrument. The input device may be selected by clicking on the required name or by typing the name in the box. The devices available on pulse-counting and analogue analysers are shown in Table 5.1.

Input device	Pulse-counting analyser	Analogue analyser	Units
SEM	✔	✔(option)	c/s (Pulse-counting) Torr (Analogue)
Raw counts	✔	-	counts
Faraday	-	✔	Torr
Total pressure	-	✔	Torr
auxiliary1	✔	✔	volts *
auxiliary2	✔	✔	volts *
f(x)	✔	✔	-
Mux*n*	✔(option)	✔(option)	-

Table 5.1 Instrument input devices

SEM Secondary electron multiplier; the gain of the SEM is controlled by the **multiplier** voltage setting in the scan's environment and the **1st dynode** voltage (if fitted).

See Section 6.4.

This detector is standard on pulse-counting instruments and optional on analogue instruments.

Raw counts This is an alternative to the SEM on pulse-counting instruments; it reports the intensity as counts instead of counts/second.

Faraday Faraday cup detector.

This detector is standard on analogue instruments.

Total Pressure The total pressure input device configures the analyser to pass ions of all masses, thus giving an approximation of the total pressure in the system. The ions are collected by the Faraday detector. The mass selected is irrelevant when this input device is used.

This detector is only available on analogue instruments.

auxiliary1 **auxiliary2**	These are analogue inputs which can be read as a scan's input; each input has user-selectable 10 V and 1 V ranges.
	The ranges are to the power 10, i.e., range 0 represents a x1 gain ($10x10^0$ full scale, 10 V) and range -1 represents a x10 gain ($10x10^{-1}$ full scale, 1 V).
	These detectors are standard on all instruments.

Note:

The names and ranges of **auxiliary1** *and* **auxiliary2** *may be configured in the Status tab.*

f(x)	This input device allows an input value to be calculated as a function of data previously acquired, or of another data value. Please contact Hiden Analytical Limited if further information is required.
	This detector is standard on all instruments.
Mux*n* where ***n*** is an integer between 1 and 16.	These input devices are used when an Analogue Multiplexer is used in conjunction with the IU to expand the number of analogue inputs to 16; refer to the Hiden Analytical Limited Manual number HA-085-001, "Analogue Multiplexer Manual", for further details.
	These detectors are an option on all instruments.

5.4.1 Acquisition range frame

Note:

The units displayed in the **Acquisition range** *frame depend on the input selected, see Table 5.1.*

Start x10E	This combination box contains the range used at the start of a scan. The value entered is a power of ten; i.e. if **-7** is entered, the range set is 10^{-7} Torr.
	For instruments with a pulse counting detector Start specifies the maximum number of counts counted. It should normally be left set to 7 (10^7 counts). If it is set to a lower value the instrument will measure how long it takes to acquire the specified count and calculate the c/s from the time. The time will not exceed the dwell time.
Auto Range	When selected, this allows the analyser to automatically change the range and follow changes in the input signal.
	The manner in which automatic ranging is applied can be controlled by the user, see Section 5.7.3.

Highest x10E   This combination box contains the highest range to which the input device may autorange; the entered value is a power of ten. **Highest x10E** is not applicable to pulse-counting instruments.

Note

*The **Highest x10E** value should be set to the expected maximum intensity, i.e. the pressure in the vacuum system as indicated by the vacuum gauge.*

Lowest x10E   This combination box contains the lowest range to which the input device may autorange; the entered value is a power of ten. **Lowest x10E** is not applicable to pulse-counting instruments.

Dwell Time   Defines the time used to acquire a single point in the scan. A value may be typed directly into the text box.

If the radio button marked **mS** is selected, the value in the text box will be specified as milliseconds. Note that if the instrument changes range the set dwell time will be used on the new range and this may affect the signal to noise ratio.

If the **%** radio button is selected, the value will be interpreted as a percentage of the default dwell time for that range. The default dwell time for a given system and range is contained within look-up tables in the IU's microcomputer; it is selected to give a good signal-to-noise ratio for the selected range.

Settle Time   Defines the time to allow the electronics to settle before the scan is started. A value may be typed directly into the text box.

If the radio button marked **mS** is selected, the value in the text box will be specified as milliseconds.

If the **%** radio button is selected, the value will be interpreted as a percentage of the default settle time for that range. The default settle time for a given system and range is contained within look-up tables in the IU's microcomputer; it is selected to allow adequate settling on the selected range.

When the scan has started, a "point time" is applied between each measurement; this time cannot be defined by the user. There are also other delays which contribute to the overall scan time.

Look-up tables, containing default dwell and settle times, for **Dwell Time** and **Settle Time** set to 100%, for pulse-counting and analogue analysers are given in Section 10.5.

Auto Zero   When selected, this forces the analyser to perform an automatic zeroing function at the start of each scan. This corrects any errors due to amplifier offsets and leakage currents.

Faraday detector

Mode	MID & PROF			BAR			BAR, log mode		
Range (Torr)	Settle (ms)	Point (ms)	Dwell (ms)	Settle (ms)	Point (ms)	Dwell (ms)	Settle (ms)	Point (ms)	Dwell (ms)
10^{-10}	2000	4	100	2000	2000	960	6000	6000	4800
10^{-9}	1000	4	80	1000	1000	960	5000	5000	4800
10^{-8}	200	4	40	200	200	160	1000	1000	800
10^{-7}	6	4	20	6	6	80	30	30	400
10^{-6}	6	4	20	6	6	12	30	30	60
10^{-5}	6	4	20	6	6	12	30	30	60

Mode	Total Pressure			Total Pressure, log mode		
Range (Torr)	Settle (ms)	Point (ms)	Dwell (ms)	Settle (ms)	Point (ms)	Dwell (ms)
10^{-10}	1000	1000	960	5000	5000	4800
10^{-9}	200	2000	160	1000	1000	800
10^{-8}	6	6	80	30	30	400
10^{-7}	6	6	12	30	30	60
10^{-6}	6	6	12	30	30	60
10^{-5}	6	6	12	30	30	60

Figure 10.25 Default Settle and Dwell times, analogue analyser, Faraday detector