MASSPORT

(VERSION 3.2)

PROGRAMS FOR THE DYCOR PORTABLE MASS SPECTROMETER

J E Patterson

School of Earth Sciences
Victoria University of Wellington

Email: john.patterson@vuw.ac.nz

CONTENTS

page

SUMMARY

This manual documents a program which controls and captures data from a DYCOR portable mass spectrometer. The program extends the capabilities of the Dycor mass spectrometer, especially in the field of thermal analysis.

You can record and view, mass spectra and their differences. You can record and view multiple ion plots, versus time. You may add a Fluke 45 digital voltmeter or a Taupo data logger, or use either independently, to record other variables. I can add drivers for other devices on request.

As many as 12 ions may be recorded and displayed as a function of time. The Taupo data logger adds 12 more inputs for a total of 24. Up to 16 Taupo logger inputs may be used if fewer ions are recorded. Displays can be re-scaled and presented in linear or logarithmic form. Ion plots may be differentiated, integrated or averaged. You can also view negative data.

A new feature allows you to continuously record full mass spectra and elapsed time.

The data files load directly into modern spreadsheets (e.g. Microsoft Works) and are easily imported into older ones.

If you record an unidentified spectrum, the linked mini mass spectral library permits searching and display of 72 common mass spectra. You can create an external library of mass spectra by running known compounds or you can type in data from standard tables.

An editor is included for file examination, correction, heading changes, adding to the library etc.

INTRODUCTION

Small, computer controlled mass spectrometers are finding many uses in science and industry, especially where processes need to be monitored or gas mixtures need to be identified.

The program described here requires an IBM compatible computer preferably with two serial ports.

A DYCOR mass spectrometer with a 1 to 100 mass range is required.

The program allows you to:

* Record a bar mode mass spectrum and display it.
* Subtract two mass spectra and display the differences.
* Record and display multiple ion plots for 12 different masses.
* Record and display 12 ion plots plus two inputs from a Fluke 45 dual display multimeter.
* Record and display 12 ion plots plus up to 12 inputs from a Taupo data logger.
* Continuously record full mass spectra and elapsed time.
* Record and display DVM or data logger inputs only.
* Retrieve data from disk using arrow key selection.
* Display a spectrum from a spectral library and search for matching peaks.
* Access the library from the spectrum collection and display programs.
* Load and edit a data file from disk.

Additional features include:

* A logarithmic mode to display large and small features.
* Differentiation to show changes, such as weight loss.
* Integration for total yields of a component.
* 7 point weighted averaging of data.
* Display or print signal peaks and their times.
* Magnification or reduction of plots using the ARROW keys.
* Panning of magnified plots to view features off screen.
* Single plot, with additional plots added in turn.
* Colour plots, or black and white plots to print graphs.
* Print out or display of spectrum partial pressures.
* Display sample spectrum only.
* Display blank spectrum only.
* Display difference spectrum, sample-blank or blank-sample.
* Enter your own scale factor to display features of interest.
* 72 common entries in the mini mass spectral library.
* Alphabetical or molecular weight ordering of library entries.
* Search for, and match, from 1 to 8 masses.
* Full screen editing of files with logical editor commands.
* Automatic catalogs of data file names and file headings.
* Thermocouple calibration.

EQUIPMENT REQUIREMENTS

Any IBM compatible computer with VGA (for colour), EGA, CGA, or Hercules display will be suitable. MSDOS 3.3 or higher is preferred and a coprocessor will speed up operation. Your computer should have 640k memory.

You need a correctly wired serial cable to connect the mass spectrometer and computer. Another cable is needed if a DVM or data logger used. Pins 2 and 3 should be crossed if DIN 25 pin connectors are used, as should pins 6 and 20. Additional information can be found in the Dycor manual.

I have tested the following cable connections using an 8088 PC clone and a Toshiba 1200 laptop computer. Both computers were equipped with two serial ports.

PC plug DIN 25	Dycor plug DIN 25	PC plug DIN 9	Dycor plug DIN 25
2	3	2	2
3	2	3	3
6	20	4	6
7	7	5	7
20	6	6	20

The Fluke 45 multimeter uses a DIN 9 plug as follows:

PC plug DIN 25	Fluke plug DIN 9	PC plug DIN 9	Fluke plug DIN 9
2	2	2	3
3	3	3	2
6	4	4	6
7	5	5	5
20	6	6	4

The Taupo data logger requires only pins 2 and 3 and pin 7 on a DIN 25 pin connector. The cable is usually supplied.

INSTALLATION

The program comes on a 3.5 or a 5.25 inch floppy disk. Before you do anything else, make another copy of the files. This is your working disk. Put the master disk in a safe place. If you have a hard disk, copy the working disk to a suitable directory, e.g.

```
C:                      Change to the C drive.
MD DYCOR                Make a directory on the C drive called DYCOR
COPY A:*.* C:\DYCOR.    Copy the files from the A drive to C:\DYCOR
```

If you have a directory for batch files, and a path set to this directory, then the file **M.BAT** should be altered to:

```
cd C:\DYCOR             Change directory from original.
massport                Run the MASSPORT program.
cd\                     Return to the root directory.
```

You can alter this file with the program **WRITE**. The programs can now be run from any directory.

SETTING UP THE MASS SPECTROMETER

Connect a serial cable from serial port 1 of your computer to the mass spectrometer. Turn the mass spectrometer on. Turn the filament on. You can leave the electron multiplier off for most purposes. Set up these communication parameters:

```
RS-232 COMPUTER          BAUD RATE 9600
DATA BITS 7              STOP BITS 1
PARITY NONE              PROTOCOL XON/XOFF
ECHO OFF
```

The programs will automatically set other parameters such as **DISP MODE, SCALE, CHANNEL, DWELL, TAB MASS** and **TAB DWELL**. The selected dwell settings give good quality signals for most applications. The dwell time increases for longer sampling intervals.

The mass spectrometer should adjusted for reasonable peak separation using **LO RES** and **HI RES**. The **DISP MODE ANALOG** peak positions should be centered on the scale marks by setting **HI POS** and **LO POS**. This is **important**, especially if heavier masses are observed. Fine adjustment can be made from the program using the **Set up mass spectrometer** options.

Settings should not differ greatly from the calibration printouts supplied with the spectrometer. Refer to the Dycor manual for more details.

THE PROGRAM MENU

Change to the directory containing the mass spectrometer programs.

e.g. **CD C:\DYCOR**

You may wish to make a directory under C:\DYCOR called MSDATA. This will contain your data files.

e.g. **MD MSDATA**

IF you have altered **M.BAT** (page 5) you wont need to change directories any more.

TYPE **M** then press **RETURN**. You will see:

```
<<<<<< MASSPORT 3 >>>>>>

Programs for the Dycor mass spectrometer
                by
          J E Patterson


      Enter letter to choose program

B: BARPLOT  - capture a bar mode mass spectrum
S: SPECRET  - display a recorded mass spectrum
D: DIFFRET  - subtract recorded mass spectra
T: TABDVM   - capture ion plots and DVM data
R: RETRIEVE - display recorded ion plots and DVM data
L: LIBRARY  - spectral library display and search
W: WRITE    - load and edit a data file from disk
E: EXIT     - exit to DOS


        Set up mass spectrometer

H: HYDROGEN - hydrogen peak position (m/z 2)
P: PEAK     - peak position high mass (e.g. m/z 44)
M: MULT     - turn electron multiplier on or off
F: FILAMENT - turn filament off (Peak turns it on)
```

Select a program and press its key. The selected program will start running.

When you exit from the selected program, this menu is displayed again. You can then choose another program or **E** for exit.

For the best results check the **Set up mass spectrometer** options **H** and **P**. These make sure that the peak positions are in the correct positions for recording. Other useful information is also displayed.

HYDROGEN

Total pressure, filament resistance, electron current and the low and high mass factors are displayed while hydrogen at m/z 2 is scanned. If the peak displayed is not centered on the screen, press **Esc** and enter the current arbitrary peak position (0-50). The chosen peak will be redisplayed nearer to the centre of the screen. Repeat if necessary.

PEAK

This works the same as for HYDROGEN except that you will be asked to enter a mass to scan. Choose a mass near the upper end of your scan range e.g. m/z 44. You may have to admit a standard vapour or gas to centre higher masses.

MULT

This turns the electron multiplier on or off. Typically this might give you about 1000 times the signal strength but with a noise increase of 10 times. This means you can improve the ability to detect small ion signals by a factor of about 100. A disadvantage is that strong ion signals are too large to be measured.

FILAMENT

This turns the filament off. On my portable mass spectrometer I have a switch to turn the screen off as this saves battery power. I prefer to turn the filament off before shutdown and, since I can't see the screen, I use this command.

BARPLOT

Pressing **B** from the menu will run **BARPLOT**. The following shows the opening screen:

```
                    DYCOR MASS SPECTRUM CAPTURE PROGRAM

                                J E Patterson

     This program accepts bargraph data from the  mass spectrometer
     and plots it on the screen.  Data is saved on disk in a format
     suitable for use in spreadsheets or for printing.


     The following commands are available:

     ARROW KEYS (UP and DOWN) - rescale spectrum.
     PAGE UP, PAGE DOWN - change scale step size.
     SPACEBAR - rescale spectrum by entering scale factor.
     L - log or linear spectrum.    H - help menu display.
     A - append data to file.       Ctrl A - automatic append.
     P - display partial pressures. Ctrl P - for printer.
     1 - get library program.       2..8 - library search.
     E - load external library.     Ctrl E - append to ext. library
     C - change search method       M - Mend spectrum after search

Press SPACEBAR to continue or ESC to exit
```

When the **SPACEBAR** (or any other key, e.g. **RETURN**) is pressed the screen is cleared you will see this message momentarily:

```
                    Serial port 1 Dycor ready
```

If the mass spectrometer is not correctly connected or is not turned on:

```
                    Serial port 1 Dycor not ready
```

is displayed briefly and then the main menu. In this case correct the fault and retry. If you succeed you will see:

```
          Enter disk drive (e.g. C:) to store data on  _
```

You may enter a disk drive e.g. **B:** or if you have a hard disk a path command such as **C:\DYCOR\MSBAR**. This path command needs to be terminated with a **"\"** if the full directory is to be displayed.

Note that continuous scanning is disabled within this program. It is enabled when you exit **BARPLOT**. This is another power saving feature for portable operation.

A WORD ON DIRECTORIES

If the directory entries occupy more than the full screen, then you are in trouble, since not all entries can be displayed at once. Large directories should be subdivided according to, sample type,

experiment series, or date, etc. This will make file searching much easier. You will also reduce the risk of choosing an existing file name for recording over.

When you enter the disk drive or path, you will see a screen like this:

```
        .   <DIR>          .   <DIR>      AIR.BAR       AIRTURBO.BAR
ALLTECH .BAR       BVACTURB.BAR       CONTAIN1.BAR      CONTAIN2.BAR
STD6657 .BAR       STD6754 .BAR       T6754   .BAR      TDSSSTD .BAR
AIR0905 .BAR       ABS4    .BAR       TEST    .BAR
 88064 Bytes free

Enter filename to store data (e.g. airsamp2): _
```

Only files with the suffix **.BAR** are displayed. Check the list of files and enter a **NEW** file name, e.g. **TEST2.BAR**. The extension **.BAR** is automatically added if it is not provided. The following screen is then displayed with space for a three line heading:

```
               Enter name or description of data:
 ------------------------------------------------------------
 Stack air sample 2, taken near top. 11/9/91.


 ------------------------------------------------------------
```

You may enter a description of the experiment. The first 25 characters will be displayed in the graph heading. If more than one line is to be entered, just keep typing, **DON'T PRESS RETURN**. Use the **SPACEBAR** to avoid breaking up words at the end of a line. **BACKSPACE** can be used to correct errors. When you have entered the description, **PRESS RETURN**. You will see:

```
Enter highest mass not greater than 140:
```

Admit the sample to the mass spectrometer. Enter the highest mass you want to record, e.g. 100. If the computer is properly connected to the serial port of the mass spectrometer a mass spectrum will be displayed on the computer screen. Otherwise an error message will be displayed, after which you will be returned to the start of the program.

SPECTRUM DISPLAY COMMANDS

UP ARROW - magnifies the ion signals by 10 for each press.

DOWN ARROW - has the opposite effect.

PAGE UP and **PAGE DOWN** - change the rescale step size from the default of 10 times. The minimum is 1.1 times. Each press increases or decreases the step size by 1.

SPACEBAR - displays this message as part of the spectrum heading:

```
Enter factor (e.g. 1e-7):
```

Enter a value as shown. This is useful where spectra are to be compared at the same total pressure.

L - gives a logarithmic display so that large and small peaks can be seen together.

H - displays a help menu to remind you of these commands.

A - appends data to your chosen filename with a ".APP" extension. Several spectra of a changing process can be accumulated for later examination. Any trends may be examined using a spreadsheet.

Ctrl A - continuously appends data to your chosen filename with a ".APP" extension. Elapsed time in minutes is logged in column 1. The interval between samples lengthens as the file gets larger. This command is only active in **BARPLOT**.

P - displays partial pressures on the screen.

CTRL P - prints partial pressures on the printer.

1 - Starts up the LIBRARY program. Use this command if you want to enter lines manually. For instance, it is a good idea to enter the highest significant masses in the spectrum as these may be from the molecular ions. This simplifies interpretation of spectra. If you want the external library, press **E** first.

2..8 - library search. Choose a number e.g. 4. The 4 strongest lines are searched for. 4 lines are removed from the spectrum for the next search. Items which persist during successive searches are more likely to be present. An 8 line search with or without **C** being pressed is recommended as a starting point. Don't expect too much as the library size is limited to 72 items.

E - This loads an external library called MASSLIB.DOC which can contain mass spectra which are specific to your application. This library may be edited using WRITE and new entries added from standard libraries. The format is name, molecular weight, eight masses and eight relative intensities.

Ctrl E - This allows you to append your own spectra to the library. Use **DIFFRET** to subtract any air blank. You need to enter a name and a molecular weight. If you are not sure of this just enter the highest mass displayed.

C - This changes the search method when the library search is carried out. In this case lines grouped around the strongest line are also included in the search. For example if a 3 line search is chosen then 5 remaining lines around the strongest line are included in the search.

M - mend spectrum. This restores lines removed from the spectrum by the library searches.

ESC - will return you to the main menu.

SPECRET

To retrieve the spectrum from the disk, press **S** from the menu to run **SPECRET**. You will see:

```
                    DYCOR MASS SPECTRUM DISPLAY PROGRAM

                                J E Patterson


     This program reads bargraph mass spectrum data stored on disk
     and plots it on the screen.

     The following commands are available:

     ARROW KEYS (UP and DOWN) - rescale spectrum.
     PAGE UP, PAGE DOWN - change scale step size.
     SPACEBAR - rescale spectrum by entering scale factor.
     L - log or linear spectrum.    H - help menu display.
     A - append data to file.       Ctrl A - automatic append.
     P - display partial pressures. Ctrl P - for printer.
     1 - get library program.       2..8 - library search.
     E - load external library.     Ctrl E - append to ext. library
     C - change search method       M - Mend spectrum after search

Press SPACEBAR to continue or ESC to exit
```

Press the **SPACEBAR**. Enter the disk drive where the spectra are stored, e.g. **D:** and **press RETURN**. If the spectra are stored on the current drive then just press **RETURN**. You may see a directory like this:

```
MSDATA      <DIR> MOTF        <DIR> MSBAR       <DIR> TEST    .DAT
 88064 Bytes free
Select directory or data file.  Press SPACEBAR for all:
```

A cursor bar can be moved with the **ARROW** keys to select a file name or directory. If the directory **MSBAR** is chosen and **RETURN** is pressed the contents of that directory are displayed:

```
        .   <DIR>          .   <DIR> AIR     .BAR      AIRTURBO.BAR
ALLTECH .BAR      BVACTURB.BAR      CONTAIN1.BAR      CONTAIN2.BAR
TEST1   .BAR      TEST2   .BAR
 88064 Bytes free
Select directory or data file.  Press SPACEBAR for all:
```

Only *.BAR files are displayed. Pressing the **SPACEBAR** will display all the files in the current directory.

Use the **ARROW** keys to choose a file or another directory. If a file is chosen and **RETURN** is pressed a spectrum will be displayed.

SPECTRUM DISPLAY COMMANDS

Refer to **SPECTRUM DISPLAY COMMANDS** in **BARPLOT**.

DIFFRET

This program is similar to **SPECRET** except it can display either of two mass spectra and their differences. Each spectrum is normalised before subtraction to compensate for possible different total pressures. The following screen is displayed when the program is started:

```
                DYCOR MASS SPECTRUM DIFFERENCE DISPLAY PROGRAM

                                J E Patterson

     This program reads two bargraph mass spectra from disk and
     displays the difference mass spectrum.


     The following commands are available:

     ARROW KEYS (UP and DOWN) - rescale spectrum.
     PAGE UP, PAGE DOWN - change scale step size.
     SPACEBAR - rescale spectrum by entering scale factor.
     L - log or linear spectrum.    H - help menu display.
     A - append data to file.       Ctrl A - automatic append.
     P - display partial pressures. Ctrl P - for printer.
     1 - get library program.       2..8 - library search.
     E - load external library.     Ctrl E - append to ext. library
     C - change search method       M - Mend spectrum after search
     S - display sample spectrum.   B - display blank spectrum.
     D - display difference spectrum (Sample - Blank).
     R - display reversed difference spectrum (Blank - Sample).

Press SPACEBAR to continue or ESC to exit
```

Press the **SPACEBAR**. Enter the disk drive where the spectra are stored, e.g. **D:** and **press RETURN**. If the spectra are stored on the current drive then just press **RETURN**. The following message will be briefly displayed:

```
<<<<<<< Select sample spectrum >>>>>>>
```

Use the **ARROW** keys to choose a file or another directory. See **SPECRET** for details. If a file is chosen and **RETURN** is pressed then the following message will be briefly displayed:

```
<<<<<<< Select blank spectrum >>>>>>>
```

followed by a directory display. Use the arrow keys to select a second file and **press RETURN**. A difference spectrum will be displayed. Note that a small delta is seen at the top left when difference spectra are displayed.

SPECTRUM DISPLAY COMMANDS

Refer to **SPECTRUM DISPLAY COMMANDS** in **BARPLOT**. The following commands are specific to **DIFFRET**.

S - will display the sample spectrum only.

B - will display the blank spectrum.

D - will redisplay the difference spectrum (Sample - Blank).

R - will display the reversed differences (Blank - Sample).

TABDVM

Press **T** at the main menu. The following screen is displayed:

```
                DYCOR 12 MASS DATA CAPTURE PROGRAM
                        J E Patterson

 This program accepts tabular data from the mass spectrometer. It
 plots up to 12 selected ion currents as a function of time. If a
 second serial port is available, then a Fluke 45 multimeter or a
 Taupo data logger may be added to record millivolt signals.

     ARROW KEYS - Rescale graph.      H - help menu display.
     PAGE UP - increase step size.    PAGE DOWN - reduce step size.
     END - Pan the display right.     HOME - Reset display to left.
     SPACEBAR - enter scale factor.   R - rescale to full graph.
     G - grid, fine grid, normal.     Ctrl W - save data as *.DA1-9.
     M - maximise all plots.          O - remove or restore offsets.
     C - monochrome or color.         B - Change background colour.
     P - display summary.             Ctrl P - print summary.
     A - 7 point weighted average.    L - log or linear.
     D - dI/dt or normal.             I - integral or normal.
     N - negative or positive.        T - thermocouple calibration.
     Enter a mass number and RETURN to plot a single ion.
     Enter S, then a number and RETURN to plot another ion.
     Press RETURN to plot all ions.

Press SPACEBAR to continue or ESC to exit
```

The program can also be used, without the mass spectrometer, for data capture. The second serial port is used for this.

When the **SPACEBAR** is pressed the computer checks its serial ports to see if the **DSR** (data set ready) pin is being used (pin 6 on a 9 or 25 pin connector). The mass spectrometer and the Fluke DVM use this pin for data handshaking. The Taupo data logger does not.

A screen similar to the following is displayed:

```
                Serial port 1 Dycor ready
                Serial port 2 DVM not ready

Press the SPACEBAR or, press T for Taupo or F for Fluke DVM.
```

Press the **SPACEBAR** or, if the Taupo data logger or the Fluke digital multimeter is connected, press **T** or **F**. After choosing an option you can enter a disk drive to store data:

```
        Enter disk drive (e.g. C:) to store data on  _
```

When you enter the disk drive or path, the directory screen is displayed. Only ***.DAT** files are displayed:

```
        .    <DIR>          .    <DIR>
CATALYST.DAT       TESTCAT1.DAT       TESTCAT2.DAT       TESTCAT3.DAT
```

```
 IONPUMP.DAT      PUMPDOWN.DAT      TESTDVM .DAT      TESTAUPO.DAT
T6544   .DAT      TDSDSTD .DAT      TEST    .DAT
 88064 Bytes free

Enter filename to store data: _
```

Enter a file name e.g. **TEST2**, and press **RETURN**. The suffix **.DAT** is added automatically.

A space to enter a three line description of the experiment is marked on the screen.

```
                Enter name or description of data:
 ------------------------------------------------------------
 Catalyst test 2nd run. 7/11/91.  300C to 25C.


 ------------------------------------------------------------
```

You may enter a description of the experiment. The first 25 characters will be displayed in the graph heading. If more than one line is to be entered, just keep typing, **DON'T PRESS RETURN**. Use the **SPACEBAR** to avoid breaking up words at the end of a line. **BACKSPACE** can be used to correct errors. When you have entered the description, Press **RETURN**. The following screen is seen if the mass spectrometer is connected:

```
  Enter up to 12 masses separated by spaces: 2 18 28 32 40 44_
```

If you have a data logger you will be asked for the number of data logger channels to read (Up to 24 - number of masses selected, but not more than 16). The data logger channels will be assigned "masses" from 501 to 516. If for example four channels are required, then "masses" 501 to 504 will be recorded. If the Fluke DVM is selected then "masses" 501 is assigned to volts and 502 to current. Since these inputs are separate, two signals may be logged.

The following timing information is also entered:

```
Enter the run duration in minutes: 120
```

and:

```
Enter the interval in seconds (not less than 11) 60
```

The suggested minimum interval depends on the number of channels logged and the run duration. If you have a slow computer then the interval may have to be increased.

The mass spectrometer is now prepared for the run. When the mass spectrometer is ready the computer will display the message:

```
                    Writing Data .............
```

and after a delay you will hear a beep and see:

```
                  Press the SPACEBAR to start run.


   Ctrl R: restarts run.  I: increments 10 min.  D: deletes 10 min
     L: toggles log plot.  Up and down arrow keys: rescale graph
```

The following commands apply only during data capture:

Ctrl R - allows you to restart the run without having to retype the setup information. The currently displayed data is removed and the data collection restarts.

I - adds 10 minutes to the duration of the run. Repeat if needed.

D - deletes 10 minutes from the run duration each time it is pressed.

These commands don't take effect until the next sampling cycle.

L - toggles a log or linear graph display. See **GRAPH DISPLAY COMMANDS**.

Up and Down Arrow keys. See **GRAPH DISPLAY COMMANDS**.

When the **SPACEBAR** is pressed the program starts collecting data and displays it graphically. It will stop at the end of the selected duration or soon after the **ESC** key is pressed. A file called BACKUP.DAT will be created which contains a second copy of the data.

The graph may be rescaled vertically at any time. You may find that only part of the graph is redrawn or the screen blanks. This can happen when computer is reading the mass spectrometer data. The screen redraw will resume when the data has been collected.

If you have a slow computer the graph may never be completely drawn if the interval between samples is too small. This does no harm to the stored data. If you have an XT computer, add an 8087 coprocessor. This will greatly speed up graphics operations.

Many of the following graph commands are disabled during data capture. They are enabled when data collection is finished.

GRAPH DISPLAY COMMANDS

ARROW KEYS - Rescale graph during or after run, **RETURN** resumes autoscaling during a run. The up/down arrow keys change the vertical scale while the left/right arrow keys stretch the graph laterally.

H - Display the help menu if you forget any commands.

PAGE UP and PAGE DOWN - change the rescale step size. Each time an arrow key is pressed the scale is changed by a factor of 10. Pressing the **PAGE UP** and **PAGE DOWN** keys alters this factor, increasing or decreasing it by one. The minimum factor is 1.1, which is useful for fine scaling.

END - pan the display right to view data off the screen. If the right arrow key is pressed important information may move off the right side of the screen. This key allows you to view that part of the display.

HOME - reset the display to the left end of the plot. This cancels the result of pressing the **END** key.

SPACEBAR - rescale graph by entering scale factor. Enter a number e.g. 1E-7 to change scale. If you change your mind just press **RETURN** to cancel

R - rescale data to show the full graph. It cancels the effect of the arrow keys.

G - display grid. The x axis grid marks one hour intervals. The y axis grid marks every 10 intervals. If **G** is pressed again the x axis grid marks 10 minute intervals. Pressing **G** for a third time erases both grids. Note that the dot intervals in each grid are arbitrary.

Ctrl W - saves transformed data as files *.DA1 to *.DA9. This allows data that has been smoothed, for example, to be saved as a separate file. This simplifies later spreadsheet processing.

M - maximise all plots to fit the screen. Press **M** to restore the screen. This is helpful when comparing plots and may be used with single and secondary plots.

O - remove or restore offsets. This subtracts the lowest data points from each plot. This allows traces to be scaled to larger values without the baseline moving off the top of the screen.

C - toggles black and white or color display. If you use PrtSc to print the graph from a colour screen (DOS 4 and 5) then the density of lines will vary according to their colour. Pressing **C** will change the display to black and white.

B - Changes the background colour for better viewing of some colours. Press again to restore the background colour.

P - display a summary of the data. This comprises the title, the duration, the interval and the time at which each mass had a maximum value. The information can be used to rescale the graph (see **SPACEBAR**).

Ctrl P - print the summary on the printer. Press **Ctrl F** to form feed the paper.

A - displays a 7 point weighted average. This smooths noisy data. Repeat to smooth more.

L - toggles a log or linear graph display. Use this to get an overview of the whole run. Exponential plots (e.g. cooling curves) will be linearised. Pressing this twice will automatically rescale data. Don't use this where **N** has been pressed.

D - press to display dI/dt. Repeat for a normal plot. This is useful where weight loss data is collected with a data logger or DVM.

I - press to display an integral plot. Repeat for a normal plot.

N - toggles a display of negative or positive data. Data from the data logger or DVM may be sometimes be negative. This key allows such data to be viewed. Do not use the log display in combination with this key. You can alternatively press **-** for a negative display.

T - thermocouple calibration. Enter a channel number e.g. 501. Enter a cold junction temperature (celcius). Enter a thermocouple type e.g. k. A new datafile will be created with the selected channel changed to temperatures. The data will also be displayed on the screen.

Enter a mass number then **RETURN** to plot a single ion. This can be useful where one plot obscures another.

Enter **S**, then a **number** and **RETURN** to plot another ion. This command can be repeated to add further ions to the display. This is useful where data relationships need to be viewed.

Press **RETURN** to plot all ions. This restores the full display.

Most commands, except the **ARROW KEYS**, **B, C, N** and **L**, are disabled during data capture.

Note that this program can be used with the Fluke 45 DVM or the Taupo data logger independently connected to COM 2, the second serial port, unless there is only one serial port in which case COM 1 may be used. The program will omit the steps relating to the mass spectrometer.

RETRIEVE

To retrieve ion plots from the disk, press **R** from the main menu. This will run **RETRIEVE**. The following screen is displayed:

```
                DYCOR 12 MASS DATA GRAPHING PROGRAM

                          J E Patterson

     This program reads mass spectrometer data stored on  disk and
     plots it  as a function of time.

     ARROW KEYS - Rescale graph.      H - help menu display.
     PAGE UP - increase step size.    PAGE DOWN - reduce step size.
     END - Pan the display right.     HOME - Reset display to left.
     SPACEBAR - enter scale factor.   R - rescale to full graph.
     G - grid, fine grid, normal.     Ctrl W - save data as *.DA1-9.
     M - maximise all plots.          O - remove or restore offsets.
     C - monochrome or color.         B - Change background colour.
     P - display summary.             Ctrl P - print summary.
     A - 7 point weighted average.    L - log or linear.
     D - dI/dt or normal.             I - integral or normal.
     N - negative or positive.        T - thermocouple calibration.
     Enter a mass number and RETURN to plot a single ion.
     Enter S, then a number and RETURN to plot another ion.
     Press RETURN to plot all ions.

Press SPACEBAR to continue or ESC to exit
```

Press the **SPACEBAR** (or any other key, e.g. **RETURN**).

You may enter a file name e.g. **TESTCAT2.DAT** and the data will be displayed directly. You don't have to enter a file name. You can enter the disk drive where the data is stored, e.g. **D:** and **RETURN**. If it is stored on the current drive then simply press **RETURN**. If data files are present, then they will be the only ones displayed. Press the **SPACEBAR** to display other files and directories.

Use the **ARROW** keys to choose a file or another directory. If a file is chosen and **RETURN** is pressed a spectrum will be displayed. Note that any data logger or DVM channels will be displayed as "masses" 501 upwards.

GRAPH DISPLAY COMMANDS

These commands are the same as in **TABPLOT**.

LIBRARY

This program contains a library of 72 common volatile gases and vapours. You should use the library with discretion since there are many omissions from the list. It is a guide only.

The program can display bar graph mass spectra of all 72 entries, with the most intense 8 lines displayed. The list may be viewed in order of molecular weight or alphabetically. The lists may be alternated by pressing the **SPACEBAR**.

To display a spectrum enter the number beside its name. To return to the menu press the **SPACEBAR**.

If you wish to match a single line to the entries in the library select **1** and then enter the mass number corresponding to that line. A list of possible matches is displayed.

You can search the library more thoroughly by entering masses ordered as a descending sequence of intensities. To select this option enter a number from **2** to **8** depending on the number of lines you wish to match. Enter the masses in descending order of intensities. A list is displayed, which shows if more than 2 lines match. The best matches are named with an option to display spectra.

The relative intensities of lines are subject to amendment since not all compounds have been run on this instrument. Where a less common pumping system, such as an ion pump is used, relative intensities may also be altered. The following screen is displayed when the program is run:

```
MINI MASS SPECTRAL LIBRARY
by
J E Patterson

This library contains 72 entries, comprising the most common
gases and volatile hydrocarbons.  An 8 line mass spectrum of
any entry may be displayed or up to 8 masses  may be entered
for a library search.

Enter D to display a mass spectrum
Enter number (1 - 8) for n line match
Enter E to load external library
Press Esc to leave program
```

MASS SPECTRUM DISPLAY

Pressing **D** will display the entries in the mass spectral library in order of molecular weight. The numbers simply mark the position in the list and are used to select the mass spectrum to display. The following shows the full list.

```
 1 methane              2 ammonia            3 acetylene
 4 hydrogen cyanide     5 ethylene           6 nitrogen
 7 carbon monoxide      8 air ion pump       9 air turbo pump
10 formaldehyde        11 nitric oxide      12 ethane
13 methylamine         14 oxygen            15 methyl alcohol
16 hydrogen sulphide   17 hydrogen chloride 18 argon
19 propene             20 ketene            21 ethylene oxide
```

```
22 propane              23 acetaldehyde       24 carbon dioxide
25 nitrous oxide        26 dimethyl ether     27 formic acid
28 nitrogen dioxide     29 ethyl alcohol      30 acrylonitrile
31 acetone              32 normal butane      33 isopropyl alcohol
34 carbonyl sulphide    35 nitromethane       36 dimethysulphide
37 vinyl chloride       38 sulphur dioxide    39 methyl ethyl ketone
40 pentane              41 ethyl-ethanamine   42 diethyl ether
43 nitroethane          44 allyl chloride     45 carbon disulphide
46 dimethyl sulphoxide  47 benzene            48 pyridine
49 dichloromethane      50 krypton            51 cyclopentanone
52 cyclohexane          53 3-pentanone        54 hexane
55 vinyl acetate        56 1,4 dioxane        57 toluene
58 aniline              59 phenol             60 1,2 dichloroethane
61 cyclohexanone        62 heptane            63 methyl isobutketone
64 styrene              65 ethyl benzene      66 o-xylene
67 octane               68 chloroform         69 freon 12  CCl2F2
70 nitrobenzene         71 napthalene         72 trichloroethylene
```

Pressing the **SPACEBAR** presents the list in alphabetical order. Entering a number will display the appropriate mass spectrum. Press any key, e.g. **SPACEBAR** to return to the main menu.

SINGLE LINE SEARCH

A one line search can be carried out by entering 1. You will be asked to enter a `mass number.` Entering **32** and pressing **RETURN** displays the following:

```
air ion pump           has a 1  line match
air turbo pump         has a 1  line match
methylamine            has a 1  line match
oxygen                 has a 1  line match
methyl alcohol         has a 1  line match
hydrogen sulphide      has a 1  line match
carbonyl sulphide      has a 1  line match
sulphur dioxide        has a 1  line match
carbon disulphide      has a 1  line match

    Press SPACEBAR for menu
```

MULTIPLE LINE SEARCH

Returning to the main menu a 3 line search may be carried out. Press **3** and enter mass numbers **16,15,14**. The following output is then obtained:

```
methane                has a 3  line match
ammonia                has a 3  line match
nitrogen               has a 2  line match
carbon monoxide        has a 2  line match
air ion pump           has a 2  line match
air turbo pump         has a 2  line match
nitric oxide           has a 3  line match
ethane                 has a 2  line match
ethylene oxide         has a 3  line match
nitrous oxide          has a 2  line match
```

```
dimethyl ether          has a 2  line match
nitrogen dioxide        has a 2  line match

      The spectrum best matches methane

Press SPACEBAR for the best matches, P to plot, or ESC to exit
```

The best matches (3 lines) are shown in turn by pressing the **SPACEBAR** and may be plotted by pressing **P**.

LOAD EXTERNAL LIBRARY

E - This loads an external library called MASSLIB.DOC which can contain mass spectra which are specific to your application. This library may be edited using WRITE and new entries added from standard libraries. The format is name, molecular weight, eight masses and eight intensities separated by commas. The strongest intensity is normalised to 100. Note that **BARPLOT** can be used to add spectra to this library also with its **Ctrl E** command

WRITE

Write is a simple editor which will allow you to alter or correct data files. Adding information to the heading is a typical application. The editor has the same menu structure as **SPECRET** for selecting directories and selecting files to edit. The editor is derived from the **BORLAND Turbo Editor Toolbox** and uses the same **WORDSTAR** commands as many other editors.

When the program is run the following screen is displayed:

```
                    WRITE DATA FILE EDITOR

                         J E Patterson


     This program allows data files to be edited.  For instance,
     you may wish to change the information in the heading.

     The following are the most important commands:

     ARROW KEYS (UP, DOWN, LEFT, RIGHT) - move cursor around file.
     PAGE UP, PAGE DOWN - Move up or down one page, less one line.
     HOME or END - move to beginning or end of line.
     Ctrl and PAGE UP or PAGE DOWN - move to file beginning or end.
     BACKSPACE - delete character to the left of the cursor.
     DEL - delete character under the cursor.
     INS - toggle the insert mode on or off.
     F2 - save the file, then continue edit.
     ESC - option to save the file, if altered, then exit.

Press SPACEBAR to continue or ESC to exit
```

Press the **SPACEBAR**. Enter the disk drive where the spectra are stored, e.g. **D:** and **press RETURN**. If the spectra are stored on the current drive then just press **RETURN**. Use the ARROW keys to choose a file or another directory. If a file is chosen and RETURN is pressed it will be loaded ready for editing.

KEYBOARD COMMANDS

FUNCTION	KEYS	ALTERNATIVE
Character left	Left arrow	Ctrl S
Character right	Right arrow	Ctrl D
Word left	Ctrl left arrow	Ctrl A
Word right	Ctrl right arrow	Ctrl F
Line up	Up arrow	Ctrl E
line down	Down arrow	Ctrl X
Scroll up	Ctrl W	
Scroll down	Ctrl Z	

FUNCTION	KEYS	ALTERNATIVE
Page up	PgUp	Ctrl R
Page down	PgDn	Ctrl C
Beginning of file	Ctrl PgUp	Ctrl Q R
End of file	Ctrl PgDn	Ctrl Q C
Beginning of line	Home	Ctrl Q S
End of line	End	Ctrl Q D
Top of screen	Ctrl Home	Ctrl Q E
Bottom of screen	Ctrl End	Ctrl Q X
Goto line	Ctrl J L	
Goto column	Ctrl J C	
Top of block	Ctrl Q B	
Bottom of block	Ctrl Q K	
Jump to marker 0..9	Ctrl Q 0..Ctrl Q 9	
Set marker 0..9	Ctrl K 0..Ctrl K 9	
Previous cursor position	Ctrl Q P	
New line	Enter	Ctrl M
Insert line	Ctrl N	
Insert control character	Ctrl P	
Tab	Tab	Ctrl I
Delete current character	Del	Ctrl G
Delete character left	Backspace	Ctrl H
Delete word	Ctrl T	
Delete to end of line	Ctrl Q Y	
Delete line	Ctrl Y	
Find pattern	Ctrl Q F	
Find and replace	Ctrl Q A	
Find next	Ctrl L	
Abandon file (save if changed)	Esc	Ctrl K Q
Save and continue edit	F2	Ctrl K S
Save and exit editor	Ctrl K X	
Save to file	Ctrl K N	
Add window	Shift F3	Ctrl O A
Next window	F6	Ctrl O N
Previous window	Shift F6	Ctrl O P
Resize current window	Ctrl O S	
Begin block	F7	Ctrl K B
End block	F8	Ctrl K K
Copy block	Ctrl K C	
Move block	Ctrl K V	
Delete block	Ctrl K Y	

FUNCTION	KEYS	ALTERNATIVE
Hide block	Ctrl K H	
Mark current word as block	Ctrl K T	
Read block from file	Ctrl K R	
Write block to file	Ctrl K W	
Toggle insert mode	Ins	Ctrl V
Toggle autoindent mode	Ctrl Q I	
Toggle marker display	Ctrl K M	
Change directory	Ctrl J D	
Show version	Ctrl J V	
Show available memory	Ctrl J R	
Set undo limit	Ctrl J E	
Set default extension	Ctrl J E	
Abort command	Ctrl U	
Undo last deletion	Ctrl Q U	
Restore line	Ctrl Q L	

CONCLUSION

The programs described here are easy to use. They will expand the range of applications of the Dycor mass spectrometer.

The best way to become familiar with the program is to try it out. I have included checks for many types of errors including serial misconnections. If you find any errors please let me know so that they can be rectified.