

**An automatic comparator
and a program package for
spectroscopic wavelength
measurements.**

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An automatic comparator and a program package for spectroscopic wavelength measurements.

By Bengt Skogvall.

1 Introduction

The photographic emulsion is still in most cases the preferred medium for recording spectra in atomic and molecular term analysis. The prominent exceptions are spectroscopy at ion beams, where the low ion density necessitates photon counting, and Fourier transform spectroscopy, where the time dependence of the signal is recorded. At grating instruments with high resolution and high dispersion photographic recording is, however, the best choice for many reasons.

A disadvantage with the photographic recording is the fact that the data is not directly available for further processing, i.e. the plate has to be "measured" in a device generally known as a comparator. The output from this procedure is a list of line positions, and it should also include a measure or at least an estimate of the intensity of each line. The manual measurement of spectroscopic plates has always been a very time-consuming and demanding task, and many attempts have been made to facilitate the process.

1.1 Manual methods

The original precision method for measuring spectroscopic plates is to use a microscope with a cross-hair. A precision screw is used for moving the plate, and the position is determined by means of a linear scale and a graded drum with a vernier scale. This method has, however, several disadvantages. Firstly, the reading of the linear scale and the drum vernier is slow and error-prone, and secondly, the measurement of the position is only as accurate as the precision of the screw, which is temperature-dependent. Moreover, backlash in the screw makes it necessary always to move the plate in the same direction during the setting procedure. After the measurement session, corrections for the local screw errors have to be taken from a table and applied to the readings.

An important improvement was offered by Ernst Abbe, chief constructor for Zeiss in Jena. He used a second microscope, focused on a precision scale at the movable plate table, that could be made at a much higher accuracy than the screw. The reading of fractional parts was made by means of a spiral scale positioned in the eye-piece of the microscope. In this way, both the speed and the accuracy of the reading were improved, and the backlash problem disappeared.

Different methods for automatic recording of the line-positions have been tried over the years. A convenient solution to this problem is the Heidenhain system, which consists of two transmission gratings, a lamp and a detector element. The detector records the periodic change of transmission through the two gratings when one grating is moving with the plate table. An electronic amplifier processes the signal and presents it to the following electronics, which consists of a pulse counter with a display and a recording system.

Different devices have also been constructed for faster and more accurate setting on the line centers. We only mention the method where a small portion of the plate is continuously scanned by means of a rotating prism and a slit. A detector behind the slit records the photographic density at the plate, and the signal is displayed on an oscilloscope. This signal can then be used in different ways for determination of the line-position, e.g. by means of a "cross-hair" at the screen or through more sophisticated analog or digital electronic methods.[1]

1.2 Automatic methods

The problem that the systems mentioned above are trying to solve is the improvement of the accuracy and the speed of the measurement. Manual measurement of a spectroscopic plate with a high line density may take days to perform, and to automate this laborious task has always been desirable. The ideal solution is, of course, a fully automatic system, where the photographic density along the plate is recorded, and the lines are detected and the line positions are determined either directly during the recording or in a subsequent process.

Several such devices have been designed, including systems for two-dimensional scanning of astronomical recordings etc.[63][4] It is, however, only after the break-through of microprocessors that it has become possible to construct small, cheap and fully automatic comparators, where both measurement, recording and the subsequent data-processing can be handled by the same system.

2 A new computer-controlled automatic comparator

The measurement system described in this report consists of a modified Zeiss Abbe type comparator with a photo-multiplier tube to measure the photographic density of the plate and a Heidenhain scale to measure the position.

The system is controlled by an MPX-16 microcomputer. A number of computer programs are used to store and manipulate the data. An overview of the system is shown in fig 1.

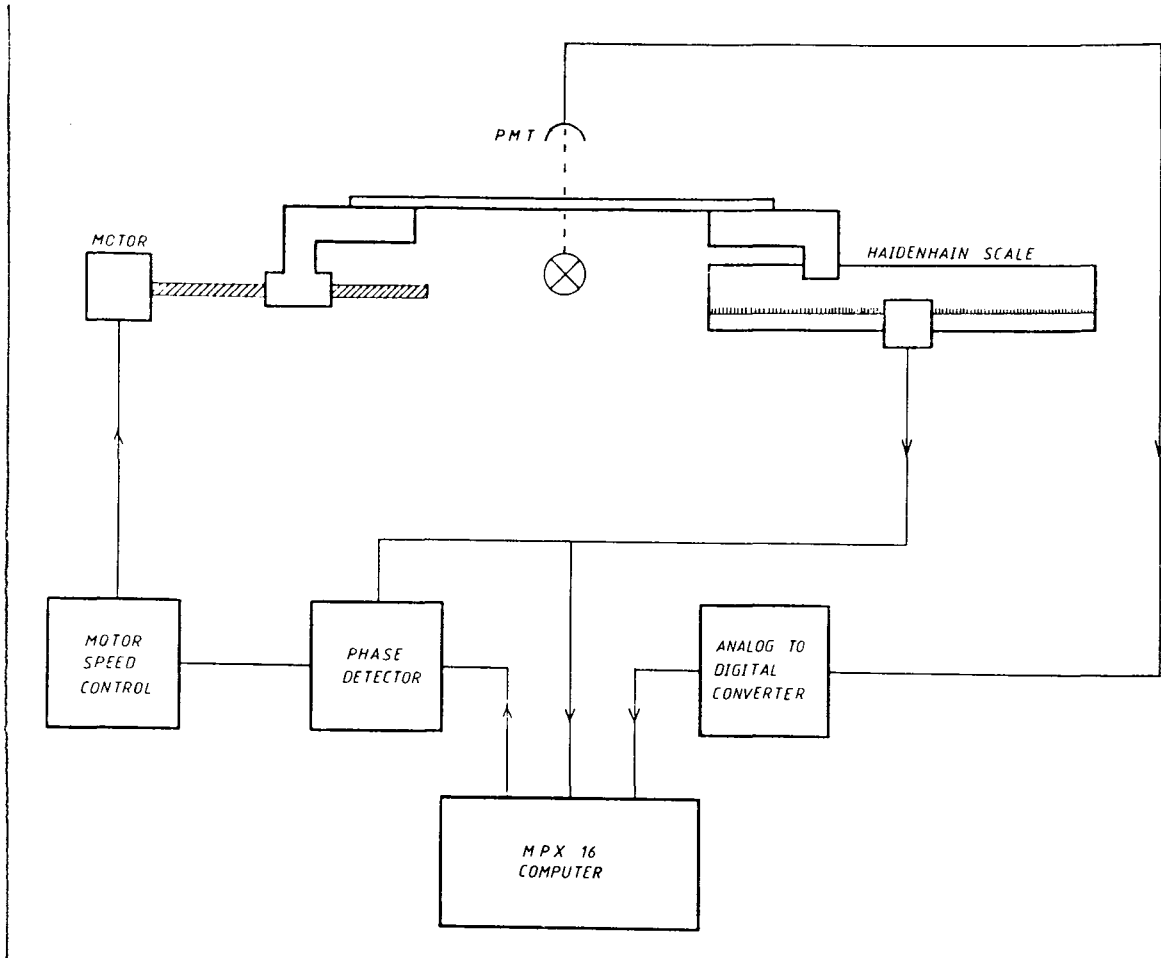


Fig 1. Overview of system.

2.1 The comparator

The comparator is a modified Zeiss Abbe instrument. A small portion of the plate is illuminated by a lamp and condenser system, and an image of the plate is focused by a microscope objective in a plane containing an adjustable slit. A photo-multiplier behind the slit measures the transmission of the plate. These modifications, shown in fig 2, are identical to those described by Gunnvald [2]. The rotating prism shown in the figure is used for scanning the plate during the adjustment procedure, when the focussing of the microscope and the optimum width, length and tilt of the slit are found by viewing the signal from the photo-multiplier tube on an oscilloscope screen.

After the adjustment procedure, the rotating prism is locked in its transmitting position and the measurement procedure is started. This is achieved by means of a computer controlled DC motor driving a precision screw, which is coupled to the comparator table through a ball nut. The output from the photo-multiplier tube is fed into the computer during the scan.

The second microscope and the scale of the Abbe comparator have been removed, and this part of the comparator table contains the Heidenhain measurement system with a scale having the accuracy of $1 \mu\text{m}$. Also the pulses from this system are fed into the computer.

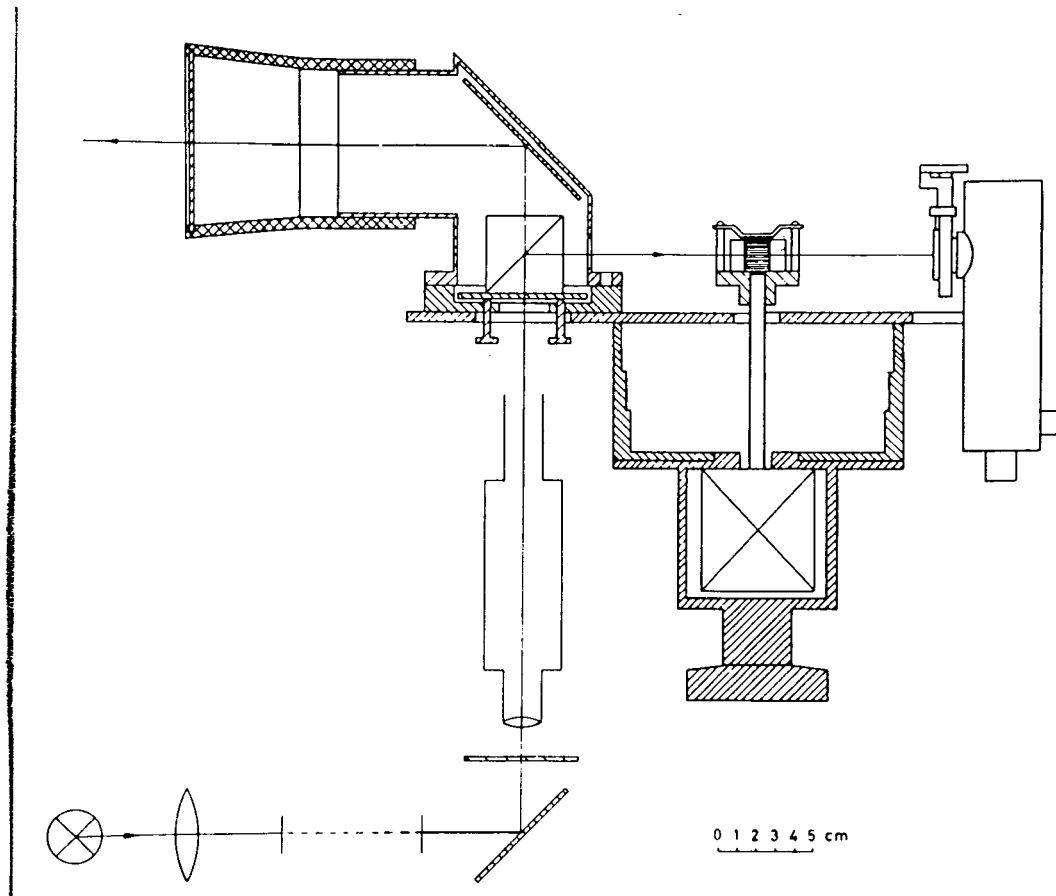


Fig 2. Abbe comparator modified according to Gunnvald.

2.2 The computer

An MPX-16 computer from Micromint Inc is used for controlling the comparator as well as for data collection and processing. The MPX-16 is compatible with the IBM PC and it is possible to run all the data-handling programs described in this report on any IBM PC compatible computer. The program to handle the comparator, however, does rely on the address of the interrupt controller, which is different in the MPX-16 compared to the IBM PC. Changing that address will make also that program run on the IBM PC.

2.3 The computer interface

The interface is wirewrapped and consists of three parts: 1)An Analog to Digital Converter (ADC) with a sample and hold circuit and a presample filter. 2)Interface circuits to decode the signals from the Heidenhain amplifier and a circuit to provide a strobe to the computer every 2 μ m. 3)A constant speed controller to select and maintain a constant motion of the carriage.

2.3.1 The ADC

The ADC is an AD574 from Intersil Inc. It features 12 bits resolution and several input ranges that can be selected by simply strapping the IC (Integrated Circuit). No calibration is needed as the ADC is used for relative measurements.

A vital thing when using an ADC is a presample filter to prevent foldback. Foldback means that frequencies above one half of the sampling frequency are, according to the sampling theorem, reduced by a multiple of the sampling frequency. For example, if we take samples at 1000 Hz, the highest frequency we can digitize properly is 500 Hz. An input frequency of 750 Hz will fold back by 1000 Hz resulting in -250 Hz, which is indistinguishable from 250 Hz. An input frequency of 1000 Hz will result in 0 Hz, which is a DC shift. Noise added in this way to the signal can never be eliminated through any kind of signal processing, so it is vital to remove the high frequency components before digitizing it with the ADC.

Another important thing is a sample-and-hold circuit. The only time this is not needed is when the signal will not change more than one half of a bit during the digitization. The AD574 does a conversion in less than 35 μ s. When using the 0 to 10 V range, one bit is equivalent to 2.44 mV. The maximum slew rate allowed is thus 0.035 mV/ μ s. When sampling a triangular wave with 10 V amplitude, the maximum frequency that can be sampled without a sample-and-hold circuit is 1.7 Hz. The maximum frequency that can be sampled using the sample and hold is of course half the sampling frequency. As the frequencies that are being sampled by this system will approach 200 Hz, a sample-and-hold circuit is used. The sampling frequency used in this system is approximately 1550 Hz, making the total measurement time for a 20 cm plate about one minute.

2.3.2 The Heidenhain electronics

The Heidenhain electronics takes care of the amplification of the typically 1–2 mV signals from the pickup element of the detector head and presents them as TTL signals to the home-built equipment. The output of the Heidenhain electronics is a two-phase clock. The phase difference is either $+90$ or -90 degrees and this is used to determine the direction of movement. When processing the signals, all flanks are converted to very short pulses, approximately 35 ns wide, and the pulses are then grouped together either as 'forward' or 'reverse' pulses. These pulses are divided by two to provide 50% duty cycle and are used as input to the constant speed motor control circuit. A further division by 4 is done before the signal is fed to the computer via a 6821 PIA (Peripheral Interface Adapter), which is programmed to

generate interrupts on each positive flank. This means that an interrupt is generated every $2 \mu\text{m}$.

2.3.3 Constant speed motor controller

The PIA is also used to control the reference frequency generator, the frequency of which is compared to the frequency of the Heidenhain pulses in a phase-detector. The output of the phase-detector is an error-signal proportional to the phase-difference of the two input signals and is fed to a PI-controller (proportional and integrating), which is the heart of the constant speed motor controller. The phase detector is taken from a 4046 CMOS PLL (Phase Locked Loop) and the PI-controller consists of two OP-amplifiers, the latter driving a Darlington transistor which, in turn, controls the current to the DC motor.

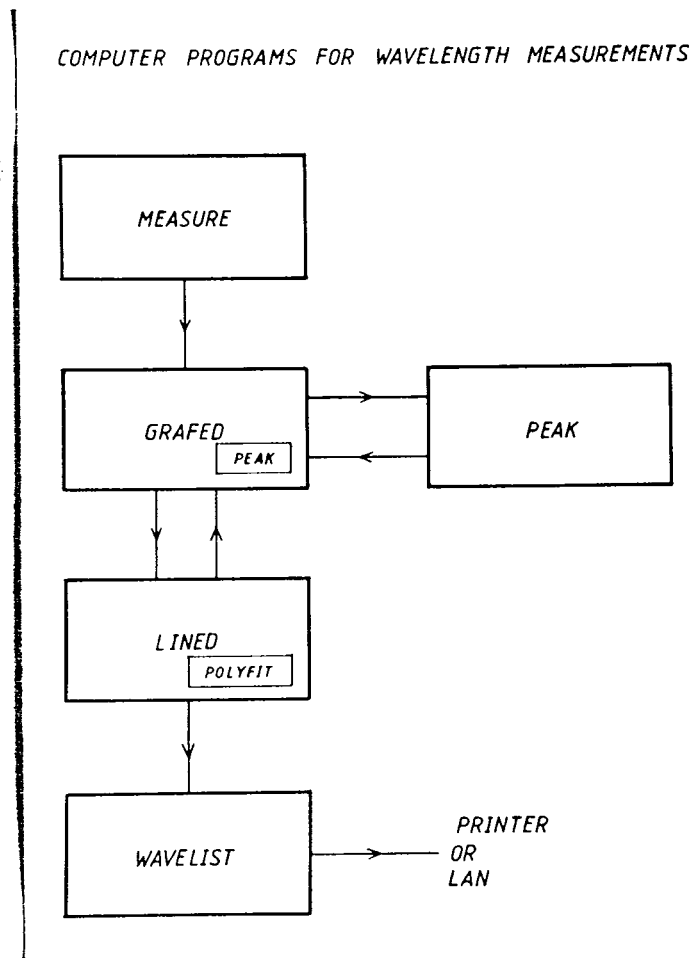


Fig 3. Overview of programs.

3 Software

One of the main objectives when the software was designed was to make the system as 'user friendly' as possible. To achieve this goal, the programs were made interactive to enable the user to get optimum performance of the system.

One characteristic feature of this program package is that the data is packed as much as possible. There are two reasons for this. Firstly, it is much faster for a micro-computer to access packed data than text-files. Secondly, it is also necessary, since saving data as text files, would overflow the 360 kBytes available on one diskette.

The programs are all written in Turbo Pascal from Borland International. Pascal was chosen for speed of development and ease of writing and maintaining as well as for packing the data as efficiently as possible. Appendix 1, section 8 contains an overview of the various formats used in this package. Fig 3 shows a graphic overview of how the programs are used.

The first program to be invoked by the user is called MEASURE. It controls the measurement process, digitizes the output voltage from the photo-multiplier tube and stores the results on an MS DOS diskette.

After the measurement it is necessary to check the recorded data. This is most easily done using GRAFED, a graphics editor. The data is plotted onto the screen, one screenfull at a time (corresponding to 1.2 mm of the plate) and checks can be made to ensure that the data has been properly recorded. The background is calculated and trial peak-findings can be performed on one screenfull of data, with varying values for certain parameters. It is very important to do this, since the result of the peak-finding depends very much on the setting of these parameters.

When the optimum settings have been found, the program PEAK is used to do the complete peak-finding of the whole recording. GRAFED can then be reentered, to check the result of the peak-finding. It is now possible to delete lines, insert new lines and to move lines, as well as comment lines and mark lines as references. If a hard-copy is desirable, PRSPEC will plot the spectra on an Epson FX-80 printer marking all the line positions found by PEAK.

A listing of all lines can be obtained using PRPEAK. This in conjunction with the spectrum-plot can be valuable when selecting reference lines for the wavelength determination.

To edit the lines found using PEAK and GRAFED and to calculate their wavelengths. LINED, the LINE EDitor, is used. This program is a mixture of a text editor and a spread sheet. For each line there are several fields where data is shown or can be input. The position of the line, in mm, from the starting point of the recording, the intensity and error-flags (to be discussed below) are some examples of data shown. Reference wavelengths and comments are examples of data that can be input. A special field shows the calculated wavelength. This field is only active when at least two references have been input and a polynomial fit has been performed. It is possible to choose to view all the lines or references only. When viewing only the references, an extra field is displayed, showing the discrepancy between the calculated wavelength and the reference wavelength.

When several measurements have been made, it is desirable to combine them into a single list of wavelengths. This is performed by WAVELIST. Wavenumbers are also calculated, with the application of Edlén's formula for the refractive index of air, if the spectrum was recorded in air.

The end product of this software package is a list of lines with both the position of the line, the wavelength, the wavenumber and the intensity as well as optional comments. Wavelengths and wavenumbers can be obtained in different grating orders.

4 Peak-finding

When a spectroscopic plate is measured manually, the cross-hair is positioned at the most dense part of a line. One way to get similar results with an automated algorithm utilizes the derivatives of the input signal. Deriving the signal, however, increases the noise, as a derivation is equivalent to a high-pass filtering. To alleviate this, the data-points are first filtered using a digital low-pass filter of user selectable degree before the derivations are performed. This digital filter is called a Hamming-window.

The most dense point of a line is of course where the first derivative is zero. As in minimum-maximum problems, it is also necessary to check the second derivative for a negative value, to ensure that it is a maximum and not a minimum that has been found.

It turns out, however, that it is more convenient to use the negative value of the second derivative as the basic criterion for a line, than it is to monitor the first derivative for zero readings. This also reduces the effects of noise. The second derivative must be less than a preset value for the data-points to be accepted as part of a line. In order to further reduce the effects of noise, the user must prescribe how narrow a line may be by setting the minimum number of adjacent data-points in a line.

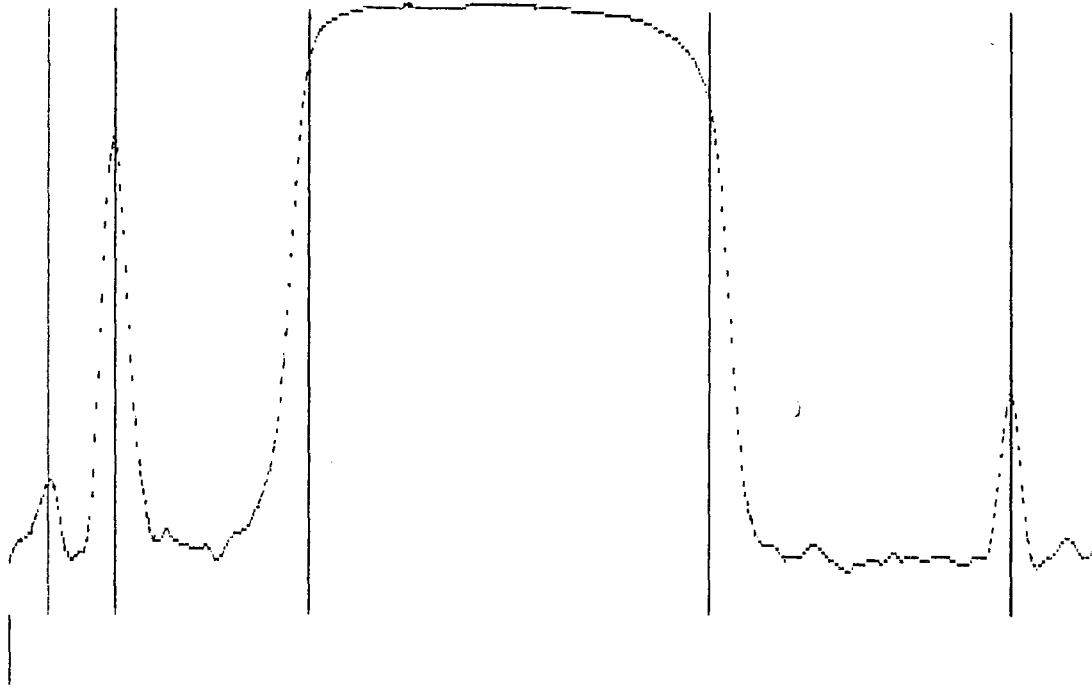
When a set of data-points has been accepted, a least-squares fit of a straight line is applied to the first derivative, and the position of the spectral line is said to be at zero-crossing of that fitted line.

The procedure above works well for lines that are symmetrical. However, for a line, which is very close to a more intense one, the first derivative may not have a zero-crossing between the beginning and end points defined by the second derivative. The position of the line is then said to be at the lowest part of the second derivative, which is calculated by taking the third derivative and finding the zero-crossing in the same manner as with the first derivative.

The spectral plates have a limited blackening range, and the strongest lines are generally overexposed. The profile of strongly overexposed lines can be said to be rectangular, which will make the peak-finding algorithm find two lines, one at each 'corner' of the line, see fig 4a, 4b. At such gross over-exposure, the position of the line is calculated as the average value of the two false ones. It is, however, important not to average two real lines, and certain conditions must be fulfilled before the averaging process takes place. Thus, the second derivative may not become more positive between the lines than a preset small value, and the relative intensities of the two lines may not differ by more than a certain amount.

31.688mm

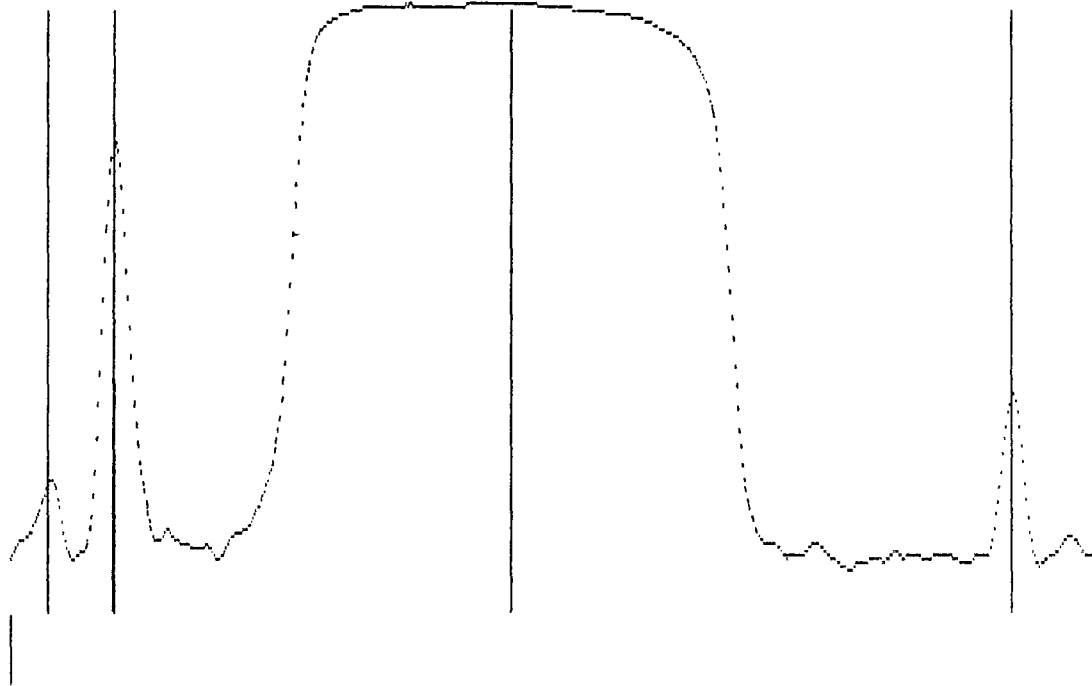
F18 = Help



a. No averaging.

31.688mm

F18 = Help



b. With averaging.

Fig 4a,b. Peak-finding of overexposed line.

Plates taken for spectroscopic term analysis are not suited for accurate intensity measurements, as generally, a large number of the lines are overexposed. It has therefore been considered not worthwhile to implement any sophisticated routines for the measurement of the intensity. The intensity of a line is simply calculated as the reading at the peak of the line minus the background times the number of accepted data–points. This value is divided by the dynamic range (total blackening – background) to make the intensities independent of the setting of the background on the comparator. For averaged lines the intensity is given as the reading in the averaged position minus the background times the distance between the two 'corner' lines plus one half of each line–width. Here, too, the value is divided by the dynamical range.

When the spectral lines differ from the ideal shape, it is important to make notes of this. Slanted lines may contain more than one line and wide lines may correspond to another element or ionization stage. When two lines are too close together, the accuracy is reduced, and so on. The slant–value of a line is calculated as the quotient of the first derivative at the beginning and the end of a line as defined by the second derivative. For ideal lines this value should be close to -1 . Deviations from -1 result in the comment of L or R, if the line is slanted to the left or the right, respectively. If the line is situated in the slope of another more intense one, S, for satellite, is printed. To get a measure of the width of a line, the number of data–points in the line is divided by the intensity of the line. When this is above a preset value, a W is printed in the comment space. The criterion for unresolved lines is that the distance between two lines should be less than a user selectable quantity, resulting in a U being printed.

5 Wavelength–determination

One of the difficult problems, in the measurement of a spectroscopic plate is to find and select good reference lines. The classic way of doing this is to first find two or three strong lines on the spectroscopic plate, measure their position with a ruler and use them to establish a preliminary wavelength scale. A polynomial fit can be performed in order to find other, not so strong references. If the first lines are correctly identified, new lines can be found. If not, the procedure has to be restarted. When fainter references have been found it is often desirable to discard the most intense ones, because the accuracy of measurement is reduced on very intense lines. This is repeated until enough references have been found, after which the final list of wavelengths is stored for further processing. When doing this manually or using non–interactive computer programs, the above can be rather time–consuming.

LINED has been designed to reduce the time spent trying to find references as much as possible. When the result of the wavelength determination is a text file, this file has to be examined either by using a text editor or by printing it. LINED solves this problem by allowing the user to perform the polynomial fit within the same program that is used to view the result. In order to make it possible to calculate new values and to show them on the screen, while still retaining the flexibility of the text–editor for viewing the results, LINED was designed as a mix between a spread–sheet and a text–editor. Thus, there are fields showing the line–position, the intensity and the error–flags that are produced by the PEAK program. There is one field where a reference wavelength can be input and another one where comments

can be added. Yet another one shows the calculated wavelength. Each spectroscopic line occupies one line on the computer monitor. It is possible to move between the lines using the same commands as when moving around inside a text-editor: The arrow-keys move the cursor one field in any direction, Page Up and Page Down move the cursor one screenfull up or down, respectively, and so on. It is possible to move to a specific line, referencing it by either its number, its x-position or its wavelength.

After inputting a number of references it is desirable to see how closely they fit. This is done by selecting to display only the references. In this mode, a new field emerges: 'Obs-calc', where the deviation between the calculated and input reference wavelength is shown. This mode is very useful and saves a great deal of work when selecting which references to discard. All this combines to make an easy to use, yet very powerful, system, where a spectroscopic plate can be processed in less than one hour.

6 References

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3. Hoekstra R., Applied Optics, 6, 807, (1967).
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Appendix 1

User's Manual:

1 Introduction

1.1 What this package does

This package of programs is designed to be used in conjunction with a comparator to measure spectral plates and to determine the wavelengths of the peaks.

1.2 Getting started

The system-diskette contains all the programs that are necessary to start and use the system. Insert the diskette in the top disk-drive, close the door and switch on the power. After a couple of seconds, the operator is asked for the date and time. The date is input as month-day-year. It is only necessary to input the last two digits of the year. The time is input as hours:minutes in the 24-hour format.

The diskette to store the data on is put in the lower disk-drive (called b:) and must be formatted before it can be used. If it has not been formatted, do so by typing 'format b:' and press <enter> when the program asks the operator to insert a new diskette.

1.3 Using the programs

There are two ways to use the programs. The easiest way is simply to type the name of the program followed by an <enter>. The program will then interactively ask the operator some questions. The answers to these questions are typed and terminated by <enter>. This mode of operation is recommended for new and unexperienced operators, as the operator is guided with questions at all stages.

The second mode of operation is to specify the answer to all questions immediately on the commandline, each answer being separated by a single <space>. This will reduce the amount of typing. It will also allow batch programs to invoke the programs in this package. As no questions are asked, this mode is only recommended to experienced operators. If not all questions are answered on the commandline, the remaining ones will be asked by the program as above.

1.4 Choosing filenames

When using the programs in this package, a number of files are created. The operator doesn't have to worry about this. When a program asks for a filename, only one name has to be typed. The program takes care of the rest. This poses some restriction on allowed names, however. The Disk Operating System allows a filename to consist of 1-8 characters and an optional extension consisting of a period and 1-3 characters. The extension is used by the programs to distinguish between the 6 different generated files, and may not be specified when a program asks for a filename.

Ex:

```
test      is OK
test.tst  is not
```

2 MEASURE

This program performs the measurement of the spectroscopic plate and stores the result on a diskette. The diskette to store the data on must have free space of at least 20 000 bytes per 2 cm to read (all reads are in blocks of 2cm).

Program prompt:

Response:

Filename:

See above for allowed filenames.

How many cm to read (max 20):

Not all of the plate needs to be measured. The smallest block that can be read is 2 cm and all larger blocks are all an integer number of 2cm. If a non-integer number is input a run-time error occurs.

The program displays:

```
Move the carriage to the far left position
by using the keys <- and ->.
Start the measurement by pressing <enter>.
Press cntrl-C to abort.
```


Below the above displayed message, a number is displayed. This is the reading of the photo-multiplier tube (PMT). Position the carriage on a blank spot of the plate and adjust the voltage to the filament lamp or the voltage to the PMT for a reading of approximately 550 to 650.

When the adjustment is completed, use the arrow-keys <- and -> to move the carriage to the left position of the block on the plate to be measured. Start the measurement by pressing <enter>. If, for some reason, it is desired to cancel the measurement, press cntrl-C to abort. Note: this can only be done before the measurement is commenced.

3 GRAFED

3.1 Introduction

The graphics data stored on a disk by MEASURE can be examined using GRAFED. The main use of GRAFED will be in finding the correct setting of the peak-finding parameters and setting of the error-flag parameters. GRAFED produces some files that are necessary for other programs. In fact, none of the following programs, except for PRPEAK, will work without some files produced by GRAFED.

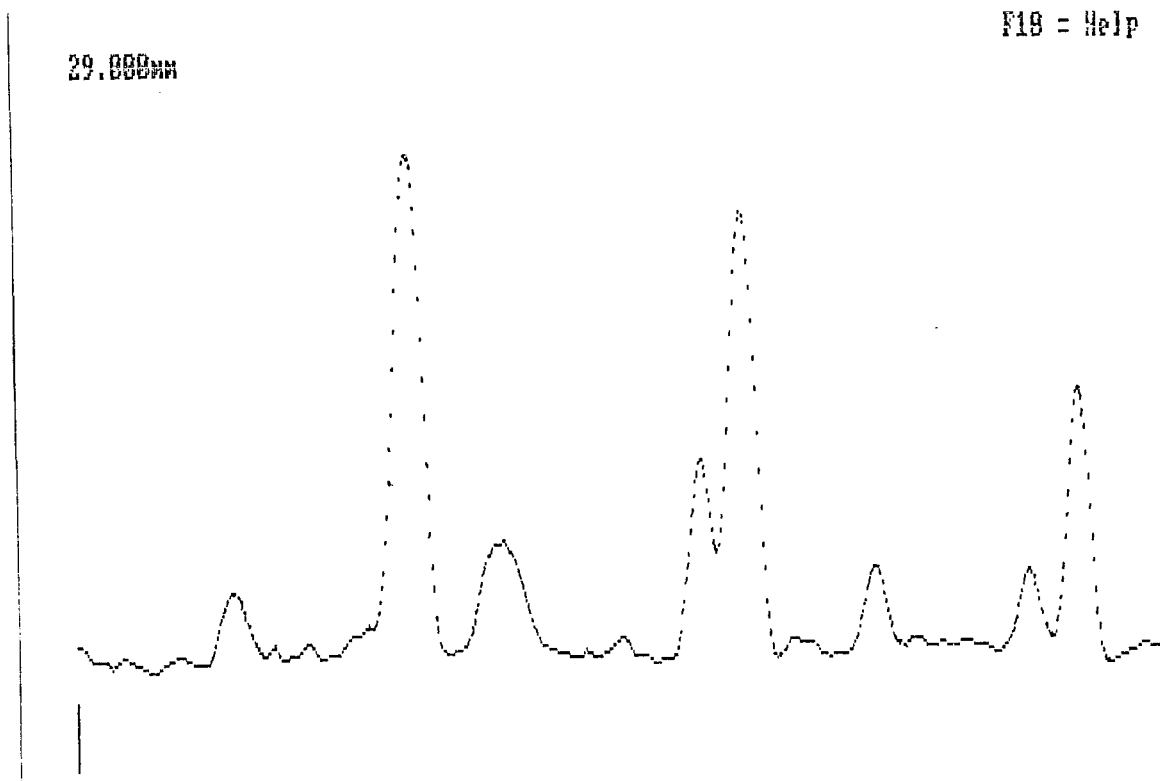


Fig 1. The display in GRAFED.

3.2 The display

Fig 1 shows a typical display. The top line is called the status line and will

contain the program prompts and the user inputs. The second line shows the position of the cursor in mm. The rest of the display is used to plot the data and the cursor, which is a vertical line at the bottom of the screen. The other vertical lines show where peaks have been found.

3.3 Moving around

The main way of moving around the measured data is frame by frame. The keys 'Pg Up' moves the display by one frame to the left and 'Pg Dn' by one to the right. The position of the cursor on the frame remains constant. At the top left of the display the position of the cursor is shown.

For faster movement 'f9' moves the left-hand side of the display to a new position specified by the operator. The unit is mm's and any real number is accepted by the program. If an out of bond value is entered the operator is notified hereof and prompted to press enter to continue.

The cursor can be moved by pressing → and ←. If the cursor reaches the end of the display, a new page is shown. For faster movement of the cursor, press cntrl and → or ← simultaneously. This moves the cursor 10 steps at a time.

3.4 Selecting plotmode

When PEAK has been executed or lines have been stored with GRAFED, all stored lines will be automatically displayed. To inhibit this, press Alt-f4. To reselect it, press cntrl-f4.

3.5 Selecting color

When using a color monitor it is possible to make it display one color and black. To select the color, press Alt-f10. The new color is selected from the table below:

0 Black	8 Dark Gray
1 Blue	9 Light Blue
2 Green	10 Light Green
3 Cyan	11 Light Cyan
4 Red	12 Light Red
5 Magenta	13 Light Magenta
6 Brown	14 Yellow
7 Light Gray	15 White

3.6 Calculating background

In order to calculate as accurate intensities as possible, it is necessary to subtract the background. The background is calculated by finding the minimum blackening in every 2 mm segment on the plate. These values are displayed on the screen as dots and over one of these dots is a vertical bar. This bar is the cursor. As it is likely that one or several of the 2 mm segments have not contained any background, these values can be edited. The usual way to eliminate such false values is to replace them with the average value of the two neighbors. This is done by moving the cursor to the dot to be averaged and by pressing f4. The cursor is, as usual, moved with the arrow-keys. When the false readings have been eliminated, the rest of the data is smoothed by pressing f3. Generally, the order of the Hamming-window need not be more than 2 to make the curve smooth enough. The result of this background calculation is used to achieve more accurate intensity readings as well as to scale the display, i.e. to place the base-lined just above the cursor and maximum blackness just below the status-line. Before the background is calculated, all background values are set to 0 and the display will look compressed. To perform the background calculation press shift-f8.

3.6.1 Editing the background

The following commands are available when editing the background.

->	Move the cursor to the right.
<-	Move the cursor to the left.
^	Move the datapoint at the cursor up.
\	Move the datapoint at the cursor down.
pg up	Move the display up.
pg dn	Move the display down.
f1	Exit. Return to normal display.
f3	Perform smoothing.
f4	Perform averaging. The datapoint is replaced by the average of its two neighbors.
f10	Help.

3.7 Peak finding

The main purpose of measuring the plate is to find the position of the peaks. As there are a number of parameters that can be changed and they have a significant influence of the result, it is necessary to be able to test the result of a specific parameter setting before invoking PEAK. The peak-finding algorithm is invoked by pressing f3.

The peak-finding algorithm differentiates the signal 3 times. The second derivative is used to detect where a line begins or ends; a value less than 0 indicates a convex curve, i.e. a line.

There are 4 parameters that influence the peak-finding. The most important one is the number of data-points a good line must consist of. A too small number causes noise to be detected as lines and a too large one causes faint lines not to be detected at all.

To reduce the influence of noise, the data-points are smoothed before the peak-finding begins. The smoothing uses a Hamming filter and the order of that filter is adjustable by pressing shift-f3. A Hamming window is the digital equivalent of a low pass filter. The cutoff frequency of the Hamming window is however fixed; the only thing that can be varied is the damping per octave. The length of the Hamming window accomplishes this. A higher setting of the Hamming window will increase the damping at high frequencies. This will reduce the number of 'noise-lines' but a too high setting will cause faint lines close together to appear as one. The Hamming window is actually a weighted average with the weighing factors looking like the cosine-bell and the length selection is the number of data-points that are averaged on each side.

The third parameter that can be adjusted is the threshold value for the second derivative. The value to input is the absolute value of the value of the second derivative at the beginning and end of a line. Normally a low value of less than 5 is used. A high value reduces the number of 'noise-lines' found to some extent, but it is better to achieve this by increasing the number of datapoints instead. A high value for the second derivative will reduce the number of good datapoints and hence the accuracy of the position of the line.

When an overexposed line is run through the peak-finding algorithm, two lines are found, one at each 'corner' of the flat top of the line. The program takes care of this by checking the value of the second derivative. If no dip has been present and the intensities of the two lines are close, the two lines are merged at their average position. To determine if there has been a dip, a fourth parameter called 'Dip between two lines to be averaged' is used: the maximum value of the second derivative between the lines must be less than or equal to this parameter, or the lines will be stored as two separate lines. A small value for this parameter will make merging more difficult, a larger one makes it easier. A value close to the value of the second derivative is generally a good choice.

Program prompt:

User input:

Value for the second
derivative:

Input any positive number as
described above.

Number of good datapoints: Input any positive integer number to select the minimum width of the line.

Dip between two lines to be averaged: Input any positive real number to select how easily two lines are averaged.

Hamming filter-order(4): The size and hence the damping at high frequencies is input as an integer. The default is 4 and will be used if the operator presses <enter> without inputting any number.

When the peak-finding is completed the found lines are displayed on the screen. Lines found in this way are called "local lines", while lines found by the program PEAK (to be discussed below) are called "global lines".

3.8 Error flags

To indicate to the operator if a line was suspect and should be treated with care, a number of error-flags are set. They indicate that the line was slanted, too close to another line or broader than normal. The setting of the parameters that determine the behavior of the error flags is performed by pressing f8. The status-line displays 'Command (w,u,s,r)' and the user presses one of the keys w,u,s or r.

W means wide and an increase of that parameter increases the number of wide lines. U means unresolved and the parameter is compared to the number of cursor-steps between two adjacent lines. S means slanted and should typically never be changed. A higher value accepts more slanted lines before setting the L or R flag for slanted left and right, respectively. R means recording media and is either Air or Vacuum.

3.9 Storing lines

Every line found with this peak-finding procedure can be stored permanently by placing the cursor just beneath the display of the line and pressing Ins. This copies all the attributes of that line to a list of lines that will be stored on a disk. If Ins is pressed in a place that is not beneath a line found by the peak-finding procedure, a line is created and stored in the same list as above, the only difference being that all parameters associated with a normal line (intensity, deficiencies of the line etc) are missing. These values can be introduced later in the line-list using LINED.

3.10 Adding comments

Any line that has been stored can be commented. Position the cursor beneath the line and press **f7**. To the left of the command line, the old comment, if any, is shown and to the right, the operator is asked to enter a new comment, which replaces the old one.

3.11 Marking references

Lines that are to be used as references, can be input using **GRAFED**, though in many cases this is more easily done using **LINED**.

Press **shift-f7** and a prompt on the command-line asks the operator for the wavelength of the line. Type the wavelength in Ångström and press **<enter>** to complete the operation.

3.12 Checking lines

It is often desirable to check what error-flags a specific line has set and whether or not it is marked as a reference. Pressing **f2** displays that information on the screen for global lines and **shift-f2** displays it for local lines found using the internal peak-finding. Top left of the screen shows the optional comment and what error-flags have been set according to the following:

W = Wide.

U = Unresolved, ie two lines too close together.

L = Slanted to the Left, i.e. asymmetric line.

R = Slanted to the Right.

S = The line is a Satellite, i.e. very close to another more intense line.

M = A line that is the average of two lines.

3.13 Summary of commands

All the commands available in GRAFED are presented below.

->	Moves the cursor one data-point to the right.
Cntrl ->	Moves the cursor the data-points to the right.
<-	Moves the cursor one data-point to the left.
Cntrl <-	Moves the cursor ten data-points to the left.
Cntrl-Home	Moves the display to the beginning of the file.
Pg Dn	Moves the display one screenfull to the right.
Pg Up	Moves the display one screenfull to the left.
Ins	Inserts a line at the cursor position. If a local line is present at that location, it will be copied to the global list. Otherwise a new line will be created.
Del	Deletes a global line.
f1	EXIT: End program and save all results.
Shift-f1	QUIT: End program without saving anything.
f2	Write to the screen the comment and error-flag of the global line at the cursor.
Shift-f2	Write to the screen the error-flag of the local line at the cursor.
f3	Perform the peak-finding algorithm.
Shift-f3	Select smoothing-degree. The digital smoothing used is called a Hamming window.
Alt -f3	Erase all local lines.
f4	Draw lines from the global list.
Shift-f4	Draw lines from the local list.
Cntrl-f4	Select auto draw of global lines ON.
Alt -f4	Select auto draw of global lines OFF.
f5	Connect the cursor and the adjoining line to start the movement of that line.
Shift-f5	Disconnect the cursor and the line to end the movement of that line.
f6	Plot the unsmoothed screenfull of data.
Shift-f6	Draw the unsmoothed screenfull of data.
Cntrl-f6	Plot the smoothed screenfull of data.
Alt -f6	Draw the smoothed screenfull of data.

f7	Enter a comment to the line at the cursor.
Shift-f7	Mark the line at the cursor as a reference and enter the wavelength.
f8	Enter trip-values for the error-flags.
Shift-f8	Calculate background.
f9	New X-position. The value given will be the new value for the left-hand side of the display.
f10	Help.
Alt -f10	Color. The color of the graphics and the text is chosen as a number from 1 to 15.

3.14 Advanced topics

3.14.1 Moving a line

Occasionally, a line has been placed incorrectly by PEAK. Such a line can be moved by GRAFED. Position the cursor beneath the line to be moved and press f5. The line is now attached to the cursor and will move as the cursor moves. Pressing shift-f5 releases the line. Note: the intensity and the error-flags will not reflect the new position of the line. These values can be changed later in LINED.

If a line is moved past another line, these lines will still appear in their original order, but the x-values will reflect their new position and the lines will appear to be out of order. It is recommended that the lines are not moved past each other.

3.14.2 Controlling the display manually

To make GRAFED as flexible as possible, it is provided with several options to display the data onto the screen. The key f6 controls what is to be plotted to the screen and f4 what lines are to be shown. It is possible to display the data in four different ways on the screen.

The fastest way to plot a screenfull of data is to use the 'plot unsmoothed' mode. It is used every time a new page is selected and can be invoked manually by pressing f6. Sometimes it is desirable to get a display with solid lines between the datapoints. This makes it easier to see very sharp lines and is achieved by pressing shift-f6. It is also possible to plot the smoothed data to see the effect of smoothing. Cntrl-f6 and Alt-f6, respectively, will perform the same operation on the smoothed data as f6 and shift-f6 does.

The default for drawing the global lines is ON, which means that every time the screen is plotted or drawn, all global lines will be drawn too. This can be deselected by pressing Alt-f4. Cntrl-f4 will reenable it. It is also possible to force the global or the local lines to be drawn on the screen. f4 draws the global lines and shift-f4 the local ones.

4 PEAK

4.1 Introduction

The program to do the hardest 'number crunching' is the PEAK program. The use of an 8087 Math co-processor is recommended. The execution time for peak-finding 20 cm without the 8087 is approximately 1h30min. This can be reduced to 20min with the 8087. There are two versions of the PEAK program on the systems diskette. PEAK and PEAK87, the latter can only be used if the 8087 is installed. The user-interface, however, is identical for both versions.

4.2 Setting the parameters

The easiest way to get the correct values for the parameters is to test different settings with GRAFED until a satisfactory result can be obtained.

Program prompt:	Response:
Filename:	See above for allowed filenames.
Value of the second derivative:	Input the value found using GRAFED.
Lowest number of datapoints in a line:	Input the value found using GRAFED.
Dip between two lines to be averaged:	Input the value found using GRAFED.
Hamming filter order(0):	Input the value found using GRAFED.
In what order are most of the lines (1..5):	Input the most frequent spectral order.
Starting-point (mm):	0 is the beginning of the spectral plate.

How much of the plate do you want to do peakfinding on (mm)? ('0' is all of the plate):

Any part of the spectral plate can be searched for peaks. 0 means all of the plate.

5 LINED

5.1 Introduction

LINED is designed to make it as easy as possible to calculate the wavelengths of the lines. By inputting at least two references, a polynomial fit can be made and the wavelengths of all the rest of the lines are calculated. There are two versions on the system disk, LINED and LINEDBW, the former should only be used with a color monitor.

Measured Lines By B. Skogvall

X-value	Intens	Note	Wavl:1	Reference	Line: 0 Max: 233 Note
0.790	1330		505.2000		
1.586	813		507.3941	507.3910	0 III
1.688	1377		507.6780	507.6830	0 III
1.870	1646		508.1798	508.1820	0 III
2.683	566		510.4213		
3.071	1914		511.4932		
6.192	136	D	520.1049		
8.253	1948		525.7952	525.7950	0 III
8.529	61	D	526.5553		
9.167	102	D	528.3163		
9.322	888		528.7457		
9.545	215	D	529.3610		
9.887	1414		530.3057		
10.196	98	D	531.1561		
11.134	71	UD	533.7461		
11.668	100	UD	535.2205		
12.126	97	D	536.4845		
12.530	68	D	537.5989		
12.615	273	UD	537.8338	537.8300	

Fig 2. The display in LINED.

5.2 The display

The display consists of a heading and several columns of data with one heading each. Fig 2 shows a typical display. The data is written in green, the headings to each column in light blue and the name of what is being edited in yellow. One of the data-fields is printed in white with a red background on a color monitor and in white on a gray background on black and white monitors. This is the cursor, and it shows the active data-field.

5.3 Moving around

The basic way to move the cursor is by using the arrow-keys to the right on the keyboard. When the cursor reaches the right or the left edge of the display, it will automatically advance to the next line and to the other side of the display. When the cursor reaches the bottom of the screen, all lines move up one step and a new one is shown at the bottom of the screen. This is known as scrolling. Similarly, when the cursor reaches the top of the screen, the screen scrolls down until the first line of the datafile is reached.

For faster movement, use Pg Dn and Pg Up, which displays the following or the previous screenfull of data, respectively. It is also possible to move to a line with a specified X-coordinate. Press f9 and the status line will ask for the new X-coordinate. Alt-f9 will ask the operator for a new wavelength. This can only be used when a polynomial fit has been made. Shift-f9 will move the cursor to a new line-number.

5.4 Entering data

There are three types of fields in LINED. The first one is the text-field, which allows the operator to input and store all characters. The second type is the numeric-field. Only numbers can be stored in a numeric-field. The third one is the protected-field. The cursor cannot enter such a field and no data can be stored there.

The Intensity and Reference columns are numeric-fields. The Error flags field and the Note field are text-fields. The calculated wavelength- and the X-value-field are protected fields.

To enter new data into a field, move the cursor to that field, and type the desired data. If a mistake is made press <back-space> to correct it, or if entering the field was a mistake press <esc> to exit without changing the contents of that field. To store the new data, press <enter> or any function- or cursor-key. This exits the field and performs the operation of that function- or cursor-key.

5.5 Handling references

5.5.1 Entering new references

To enter a new reference, move the cursor to the line to mark as a reference and the column marked 'Reference'. Enter the wavelength in Ångström and press <enter> or any function— or cursor—key to store it.

5.5.2 Deleting references

To delete a reference, move the cursor to the line containing the reference to delete and press f4. The screen is updated and the reference is removed.

5.6 Polynomial fits

One very powerful feature of LINED is the ability to make polynomial fits inside the editor. This saves time by eliminating the need to save all the data, exit the program, enter a new one and reading all the data back before the polynomial fit can be performed. Pressing f3 clears the line of headings and the program asks for the degree of the polynomial. Any degree less than 10 can be chosen. When the polynomial has been calculated, previously calculated wavelengths are replaced by the new ones.

5.7 Summary of commands

The available commands in LINED are summarized below:

->	Moves the cursor one column to the right.
<-	Moves the cursor one column to the left.
^	Moves the cursor one line up.
∨	Moves the cursor one line down.
Home	Moves the cursor to the top of the page.
End	Moves the cursor to the bottom of the page.
Cntrl-Home	Moves the cursor to the beginning of the file.
Cntrl-End	Moves the cursor to the end of the file.
Pg Dn	Displays the next screenfull of data.
Pg Up	Displays the previous screenfull of data.
Ins	Inserts a line at the cursor position.
Del	Deletes the line at the cursor position.
Shift-f1	QUIT. Leave LINED without saving.
f1	EXIT. Leave LINED and save all data to disc.

f2	Switch between normal display and references only display.
f3	Perform a polynomial fit.
f4	Delete a reference. Position the cursor at the reference to delete before pressing f4.
f7	Decrease the order of a line.
f8	Increase the order of a line.
Alt -f9	Move the cursor to a new wavelength.
Shift-f9	Move the cursor to a new line-number.
f9	Move the cursor to a new x-position.
f10	Help.

6 WAVELIST

To combine several measurements, WAVELIST is used. The operator specifies the number of files to combine and the maximum deviation between lines that are to be averaged.

PRELIMINARY: The wavelengths of the combined lines are averaged. So are their intensities and their flags are OR-ed, meaning that if a flag is set in either of the files, it will be set in by WAVELIST. To the right, the wavelengths of the combined lines are printed. The output of this program is two data-files, one that is designed for further processing by programs designed to do term-analysis. The other file is a text-file called filename.LST. Examine this file with a word-processor or print it on the printer by typing 'TYPE filename.LST >PRN'.

7 Printouts

7.1 PRPEAK

The peaks found by PEAK and their x-coordinate is printed. The output consists of the X-coordinate in millimeters and a field of error-flags as described above and the intensity of the line. If any line has been commented or marked as a reference, this information is also printed out. This printout can be made immediately after PEAK has calculated the peaks.

Program prompts:	User inputs:
Filename:	See above for allowed filenames.
All lines or References only:	To make a printout of all lines found by PEAK press 'a'. To make a printout of only those lines that have been marked as references, using GRAFED or LINED, press 'r'.

7.2 PRSPEC

This program is designed to produce a hard-copy output of the graphics display shown by GRAFED. The height of the spectrum as well as the magnification of the x-axis are user selectable. A baseline is printed, and each peak is marked with a vertical bar.

The program prompts:	User response:
Filename:	See above for allowed filenames.
Baseline:	This is the position of the baseline. A value of 400 is usually good. A higher value moves the spectrum downward, and a lower one moves it upward.
No of printlines:	This is the height of the spectrum. Try 5 to start with. A higher number produces a taller spectrum.
X-scale:	1 prints every datapoint, making each line equivalent to 1.5 mm on the plate. 2 is equivalent to 3 mm etc.
Y-scale:	This value should be roughly equivalent to $(2000 - \text{baseline}) / (8 * \text{No_of_printlines})$. For a baseline of 400 and the No of printlines set to 5 the Y-scale should be set to about 40. A smaller value will increase the size of the spectrum and if a too low value is selected the

spectrum will overflow and be printed as a solid line at the top pixel.

Starting-point(mm): It is possible to print any part of the spectrum. 0 is at the beginning of the spectrum.

Length of spectrum(mm): The length should be set to one or two mm shorter than the desired printout, as the program will end any printline it has started.

7.3 PRWAVE

This program is very similar to PRPEAK, except that it also prints the calculated wavelength of each line. This makes it useful as the final printout of a measurement.

Program prompts: User input:

Filename: See above for allowed filenames.

First order to print wavelength:

Last order to print wavelength:

First order to print wavenumber:

Last order to print wavenumber:

The user may print a maximum of 4 columns of wavelengths and wavenumbers. To inhibit printing of either wavelength or wavenumber, input a last order less than first order.

All lines or References only: To make a printout of all lines found by PEAK press 'a'. To make a printout of only those lines that have been marked as references, using GRAFED or LINED, press 'r'.

8 The formats used by the programs

This section is intended for programmers who wish to write their own application programs that use the datafiles in this package.

In several places there is a need to store real values, such as the position of the peaks, their wavelengths etc. As the programs are designed to work both with and without the 8087 math co-processor and these formats are not compatible, a new type called fixed is used. It consists of a three-byte unsigned integer for the integer part and a two-byte integer for the fractional part that should be divided by 10000 before adding it to the integer part. All integers are stored with the least significant byte first.

```
fixed = record
    Integer_part:array[1..3] of byte;
    Fractional_part:integer;
end;
```

The first file created is the 'Raw DaTa file' called .RDT. It is formatted as a file of integers, low byte first. Only positive values between 0 and 2048 are used. Note: Future development of the system may change this.

GRAFED produces four new files: .PRO, .PEK, .REF and .KOM.

.PRO is a profile-file which contains a string of two-byte integers that define the background, slanted parameter, wide parameter, unresolved parameter, as well as the result of the background calculation. Some fields are marked as not used. These are kept to provide compatibility with earlier versions.

```
protyp = record
    bakgrund:integer; {not used}
    snedfel :integer;
    bredfel :integer;
    blend :integer;
    basline :integer; {not used}
    factor :integer; {not used}
    luft :boolean;
    bakgr :array[0..101] of integer;
end;
```

.PEK is the file containing the found peaks. It is formatted as described below:

```
linetype = record
    pos : fixed; {the unit is 2 microns}
    intens : integer; {intensity}
    kom : byte; {pointer to .KOM file}
    err : byte; {error flags}
    ref : boolean; {true if marked as reference}
    ordning: byte; {The order of the line}
```


end;

.REF contains the references and it is formatted as follows:

```
referencetype = record
    l:linetype; {a copy of the line that is marked}
    v:fixed;    {the wavelength in Ångströms}
end;
```

.KOM is the comment file. A maximum of 256 lines can be commented. A bytefield of 32 bytes is used to mark what is used and what is not. A logical true is used to mark the comment as used.

```
komtyp = set of byte;
kommentarer = array[0..255] of string[20];
```

```
komfiltyp = record
    ledig : komtyp; {flag set means occupied}
    kom   : kommentarer;
end;
```

.POL is the file created when a polynomial fit has been made. It is formatted as a textfile containing the coefficients of the polynomial in scientific format, the first one being the X^0 term and the last X^{10} term.

Note: when using the 8087 math co-processor to calculate the polynomial, 3 digits are allocated for the exponent. The first one must be deleted with a word-processor if the numbers are to be read by a non-8087 program.