

Appendix B: An Automated Spectroscope

B.1: Basic Requirements

The accurate measurement of weak emission line intensities places certain requirements on the measuring system:

- The system must be sensitive, or some lines may be too weak to be adequately measured.
- The noise level must be low enough to not impair measurements of the weakest lines.
- The resolution must be high enough to separate nearby lines. A higher resolution is desirable, so as to permit easier detection of any problems such as self-absorption which typically affects the profile of the spectral line.
- The light source used must be stable; the intensities of the lines produced must remain constant during the time over which the line intensities are measured.

B.1.1: Requirements for Light Source

The light source must be sufficiently stable so that the output from the light source does not significantly change during measurements. If the lines being measured are very weak, the time involved can extend to many hours, so source stability needs to be seriously considered.

The light source should also be spectroscopically pure in order to reduce the total light output (reducing the signal to noise ratio) and to reduce the occurrence of blended lines from the source.

If any highly excited lines are to be measured, the source must be capable of producing sufficiently large populations for the levels involved.

Lastly, the output from the source for a particular line must be proportional to the line strength. In practice, this depends on avoiding self-absorption.¹ Ideally, the atomic level populations in the light source would be predictable accurately, but this tends to be difficult to achieve in practice.

The best type of source to use depends on the particular elements and transitions involved, as the strength and excitation energy of the line will place restrictions on some types of source, and the element involved will also eliminate some possible sources. As the major elements of interest for the solar spectrum are the elements from titanium to nickel (Ti, V, Cr, Mn, Fe, Co, Ni), a hollow cathode lamp is particularly suitable as a source. The major drawback with the hollow cathode lamp is that the level populations are not known. This is typical of all non-LTE sources.

A hollow cathode lamp is an emission line source, with a spectroscopically pure sample of the element under investigation forming the cathode in a low-pressure inert gas discharge. The cathode has a small hole in it, with the emitting population being formed by cathodic sputtering at this hole. The inert gas ions in the discharge bombard the cathode, ejecting excited atoms from the cathode into the surrounding region, where they produce emission lines through spontaneous emission.

A hollow cathode lamp can also be configured to reduce the possibility of self-absorption. This involves producing an optically thin emission region.

B.1.2: Requirements for Detector System

Some important features of the design of the monochromator should be noted. The wavelength should be accurately controllable, to allow for easy measurement and identification of lines. The resolution should be sufficient to resolve closely spaced lines if necessary. The monochromator should be efficient, making as full a use of available light as possible, enabling the measurement of weaker lines. Scattered light within the monochromator should be kept as low as

¹Self-absorption occurs when a significant portion of the light emitted by the source is absorbed within the source, leading to a lower than expected output for the line affected. The profile of a line also tends to be altered. See section A.3.5 for a discussion on the detection of self-absorption.

possible to keep noise in measurements to a minimum. This last consideration is quite important, as not only are the actual line intensity measurements affected, but intensity calibration of the monochromator using a continuum source becomes more difficult to perform accurately.

Accurate measurements for weak lines in particular will require low noise in order to obtain acceptable signal-to-noise ratios. If the background noise is high, taking data over a longer period to obtain a stronger signal will not help matters greatly; if the background noise is low, accurate results can be obtained for weak lines simply by counting photons for a longer period.

A simple scheme to reduce the background noise within the detector system is to reduce the total amount of light entering the system by filtering the input to remove unnecessary portions of the light. Simple useful filtering can be performed by using a low-pass filter to remove shorter wavelengths to prevent the first and second order patterns within the spectrometer overlapping. A more comprehensive filtering scheme is to use a double-pass monochromator, wherein the input is passed through two monochromators, the first acting as a filter for the input to the second monochromator.

A high quantum efficiency is desirable for the photodetector in order to measure weak lines. A photomultiplier or CCD array would be a suitable detector. With a high detector efficiency, the noise levels must be low. This low noise level is the most critical feature of the spectroscope, so any low noise monochromator of adequate resolution should be acceptable.

B.1.3: Requirements for Control System

Such a spectroscopic system would be computer controlled - this allows the system to operate for long periods with minimal operator intervention and allows data to be readily viewed and processed without having to be transferred.

The control system should be simple to use and maintain. (This applies to both the hardware and software involved.) This is a basic requirement for any automated experimental system. With the low cost and readily availability of modern microcomputers, and their standardisation, there is no reason not to use such a microcomputer for the control computer.

The development of the control system is then reduced to the problem of interfacing the control microcomputer and the rest of the system, rather than the somewhat greater problem of building the entire control system. In the interests of standardisation and the ready interchangeability of parts, the computer should be able to treat the spectroscope as just another peripheral. The control system then consists of the experiment, and the software required to drive it.

The software to control the experiment is vital, and due attention should be paid to its proper development. Too high a proportion of experiment control software that is written is of poor quality; such software is frequently undocumented, difficult to use, and cryptically written. A computer controlled experiment will typically have many users over time, and changes will be made to the system. If new users can readily use the control system, their time spent with the system can be much more productive. Section B.4.3 discusses the control software for this particular case.

The typical new microcomputer is quite capable of driving such an experimental system and having plenty of spare capacity, so there is no need for the control computer to be dedicated solely to controlling the experiment. Alternately, an older computer could be readily used, providing useful employment for what would otherwise be a machine of very limited use. The computer must be capable of running the control software; this limits the software somewhat on low performance systems for tasks such as displaying data by affecting the graphics capabilities and the amount of data that can be kept in memory at one time. The total volume of data is less of a problem; without any form of data compression, a complete visible spectrum taken with a step size of 0.02\AA will be about 5 MB of data, which is quite capable of being stored on virtually any hard disk drive.

B.2: The Light Source

A hollow cathode lamp was chosen as the light source (see section B.1.1). A hollow cathode lamp meets the stability requirements and is capable of producing high excitation lines. Also, the spectra of the most photospherically desirable elements can be readily obtained from a hollow cathode lamp. Figure B-1 shows the hollow cathode lamp used.

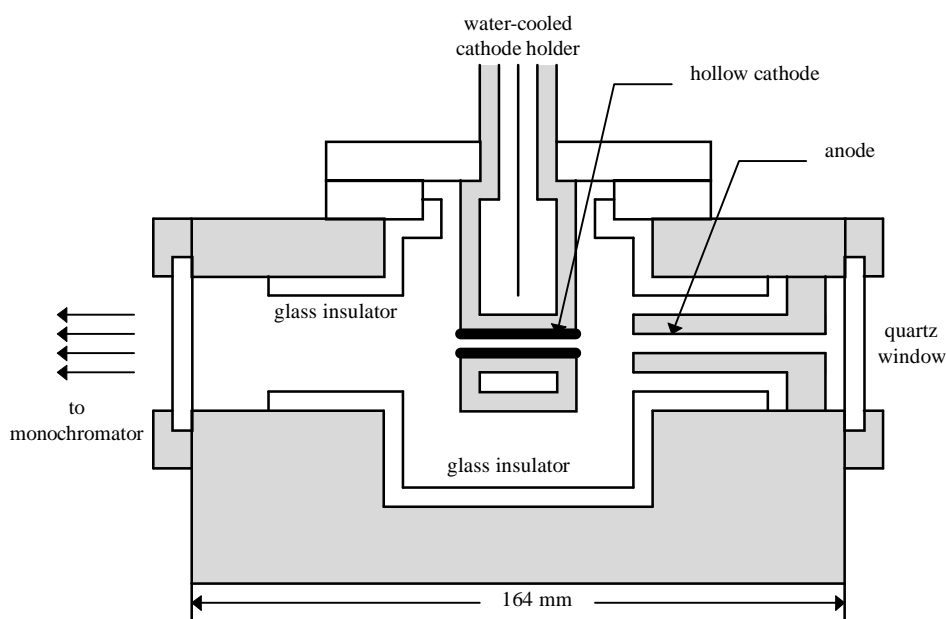


Figure B-1: The Hollow Cathode Lamp

During operation, a potential difference of about 300V is maintained between the anode and cathode. A high voltage RF potential is applied to begin the discharge. The interior of the lamp is filled with a low pressure inert filler gas (usually argon). The quartz windows allow ultraviolet lines to be measured. A light path through the entire lamp is present, allowing the introduction of a laser beam for alignment of optical components.

A hollow cathode lamp is used as when driven by a suitable constant current power supply, it meets the stability requirements needed to allow data gathering runs of long duration. In addition to this stability, the hollow cathode lamp has a number of other advantages: it produces intense lines, thus maximising the signal to noise ratio and reducing the necessary counting time; the lines produced are narrow, with the

measurement system determining the resolution obtained. With the particular design used here for the hollow cathode lamp, the element under investigation can be readily changed, and the gas used to form the discharge can also be altered. A hollow cathode lamp is also simple, safe and relatively cheap to operate and maintain.

The constant current power supply used in this experiment consisted of an unregulated supply in parallel with a smaller supply regulated so that the current passed through a resistor is constant.

The design used for the hollow cathode lamp shows a number of advantages over other designs. It can be easily cleaned and the cathode changed. This, apart from being useful in the day-to-day operation of the lamp, enables easy experimentation with the lamp to determine the optimum design, including attempting to match the hollow in the cathode to the input slit of the monochromator system by using a slit shaped hollow. The construction of an anode of variable length would not be difficult if this was desired. The lamp is designed so that the system can be aligned using a laser with the hollow cathode lamp still in place.

The water cooled cathode allows the operating current to be higher than would otherwise be possible with a non-cooled lamp. The lamp was typically run with a current of 0.25 A. A non-cooled commercial lamp is typically run at about 10 mA.

The pressure and flow rate of the filler gas are controllable, allowing the user a high degree of control over physical conditions in the lamp.

The hollow cathode lamp in this experiment is typically operated with the filler gas being argon at 0.5 - 1.0 torr, a current of 0.25 A, and a cathode voltage of 300V. The anode allows the discharge to be readily started and maintained at this pressure, without it, reliable operation would require a higher pressure. A low gas pressure, of 1 torr or lower, is best as the discharge is more stable, and the output is more intense.

The system is set up to be able to use either argon or helium as the gas in the hollow cathode lamp, with argon generally being used as it produces greater excitation of high excitation energy levels than helium, due to the higher atomic mass of argon. Argon also produces more lines than helium, causing more interference with the spectrum being investigated. If this is a problem, helium can be used instead.

The intensity of emission lines from the filler gas can be reduced by running the discharge at the far end of the cathode, with the water-cooling jacket and the cathode

masking the region where the discharge is in the filler gas only. The anode also reduces the intensity of the argon lines.

B.2.1: Level Populations in Hollow Cathode Lamps

The greatest drawback with the hollow cathode lamp as a line source is that the level populations within the lamp are not in LTE. As the atoms ejected from the cathode are excited in this process and then emit, the population of any level is determined by the initial population and by the rates at which the level is depopulated by emission to lower levels and repopulated by emission from higher levels.

The level populations will be in equilibrium state, however, as long as the excitation rate is constant. The population of a level i in equilibrium will be given in terms of an excitation rate R_i by

$$N_i = \frac{R_i + \sum_{k>i} A_{ki} N_k}{\sum_{j<i} A_{ij}} \quad (\text{B-1})$$

if no significant absorption or stimulated emission occurs. As the populations of higher levels will generally be lower than that of level i , the level population can be roughly approximated by

$$N_i = R_i T_i \quad (\text{B-2})$$

where T_i is the lifetime of level i . As the population of a level i will strongly depend on the level lifetime, as well as the spontaneous emission rates from higher levels, it will generally be impossible to accurately determine level populations. Even nearby levels will have quite different populations if their lifetimes differ significantly. A hollow cathode lamp is therefore only suitable for measuring relative intensities of lines with common upper levels.

B.3: Monochromator System

The monochromator system used to measure the line intensities is shown in figure B-2. At the heart of the system is the 3 metre Czerny-Turner monochromator.

A photomultiplier tube is currently used to detect the output from the monochromator. The tube can be cooled during operation to reduce noise levels.

A low-pass transmission filter and a second monochromator are used to obtain a suitably low background noise.

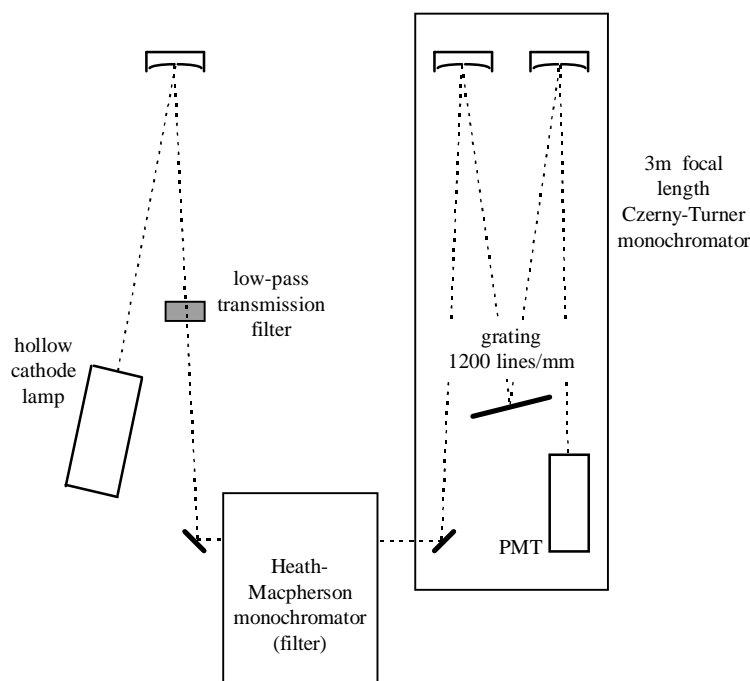


Figure B-2: The Monochromator System

The system is mounted on a heavy slab ($\approx 3t$) on vibration-damping supports. The optical components are from the monochromator system described by Milford,² with a new computer control system and hollow cathode lamp replacing those used in the old monochromator system. Further modifications are planned.

²Milford, P.N. "Line Intensity Ratios and the Solar Abundance of Iron" PhD Thesis, The University of Queensland (1987) and Milford, P.N., O'Mara, B.J. and Ross, J.E. "Measurement of Relative Intensities of Fe I Lines of Astrophysical Interest" *Journal of Quantitative Spectroscopy and Radiation Transfer* **41**, pg 433-438 (1989).

B.3.1: Low Pass Transmission Filter

A low pass filter is used to further cut unwanted light by preventing short wavelength light being passed in higher order diffraction. The particular filter in use depends on the wavelength, and an appropriate filter is selected by the control computer.

B.3.2: Band Pass Filter

The major component of the filter system used is the Heath-Macpherson 0.6 metre monochromator, which is also controlled by the computer system. This monochromator has a bandwidth of about 17\AA . This greatly reduces the background light within the main monochromator. Alterations have been made to allow the wavelength to be controlled to sufficient accuracy.

B.3.3: The Monochromator

The major optical component is the 3m focal length medium resolution monochromator. The output from the input filter system (the low-pass transmission filter and low resolution monochromator) forms the input, and the output is passed directly to the detector. The monochromator itself is a Czerny-Turner monochromator of conventional design. The monochromator and the positioning of its components is shown in figure B-3.

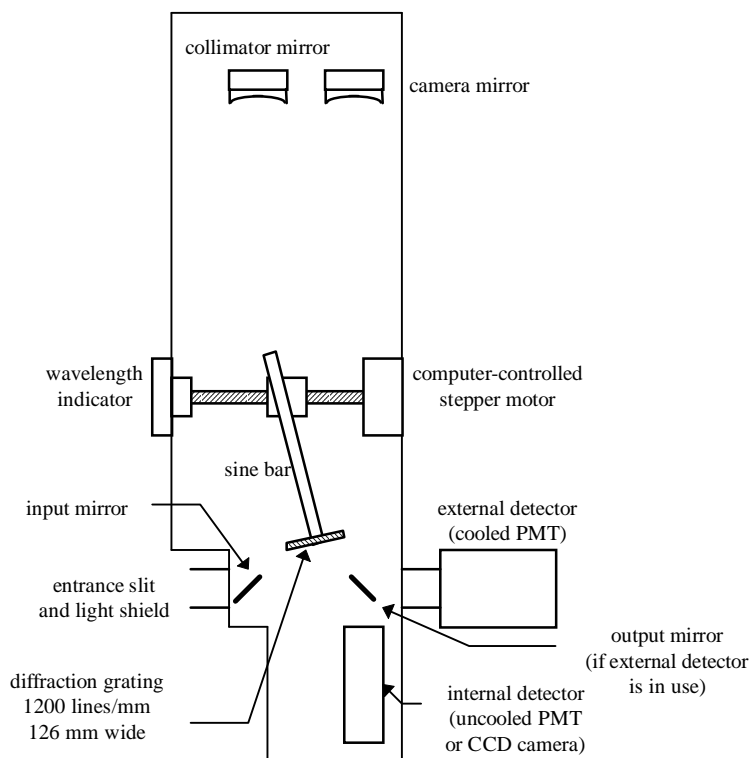


Figure B-3: 3m Monochromator

If a cooled photomultiplier tube is used as the detector, it must be mounted off the main optical bench in order to isolate vibrations produced by the cooling system.

The stepper motor and sine bar used allow the grating to be positioned with a wavelength precision of 0.02\AA . If measurements are made at successive positions, this gives a step size of 0.02\AA .

The grating blazed at 3000\AA with $1200\text{ grooves mm}^{-1}$ has an effective width of 126 mm, giving a theoretical resolution of 0.04\AA in first order. For this resolution to be fully exploited, the entire grating must be illuminated by the source. A large collimator mirror must therefore be used to direct the input towards the grating. The focal length of the mirror must be long enough to avoid excessive spherical aberration. The collimator mirror (and the identical camera mirror) have focal lengths of 2.9 m. The light path, showing the full width of the grating being illuminated, is shown in figure B-4.

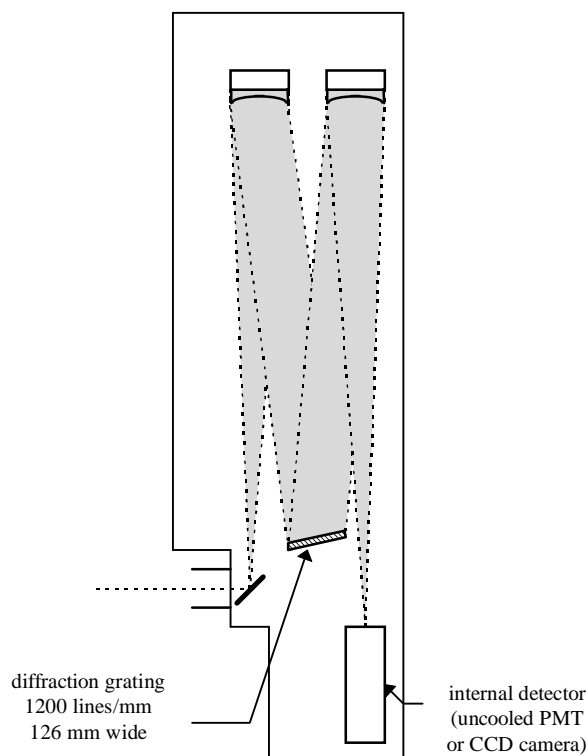


Figure B-4: Monochromator Light Path

As any light in the monochromator not on this light path is undesirable, light-absorbing baffles (not shown in figure B-3) are used to reduce stray light. The scattered light within the monochromator is already reduced to low levels by the input filter monochromator.

The dispersion of the system is $\approx 2.3\text{\AA mm}^{-1}$ in the focal plane of the camera mirror. The effective resolution of the system is thus largely determined by the detector size (the exit slit width where the detector is a photomultiplier). A wide exit slit (or large detector) can be used to increase light levels, or a narrow exit slit can be used to improve resolution. The exit slit or detector must be in the focal plane of the camera mirror.

B.3.4: The Photodetector

The photodetector currently in use is an EMI 9658A photomultiplier tube with an S20 cathode. A magnetically shielded thermoelectrically cooled (to $\approx -20^\circ\text{C}$) housing can be used to reduce the dark count rate. The output from the PMT is

passed through a pulse amplifier and discriminator, and the individual events are then counted by the control computer.

The low light levels encountered when measuring intensities of weak lines require a detector with the sensitivity of a PMT to be used. A device with such sensitivity that offers a number of advantages over a photomultiplier is a CCD camera. A CCD camera allows a number of wavelength points to be measured simultaneously, so an entire spectral line can be measured at once. The horizontal spread of pixels in the CCD array provides the wavelength variation. If a two-dimensional CCD array is used (as opposed to a one-dimensional linear array), the vertical pixels will provide multiple spectra. These spectra can be compared for errors, and can be combined to find a mean spectrum. The resolution of a CCD camera will depend on the size of the array elements (combined with the spectral dispersion of the system) and cannot be changed by altering the exit slit of the system.

The monochromator system is currently being converted to the use of a CCD photodetector.

B.4: Control System

B.4.1: The Control Computer

The control computer selected was an IBM-compatible XT. Such a computer has adequate performance for use as a monochromator control computer. Virtually any standard microcomputer for which suitable interface hardware can be obtained or constructed, and on which control software can be developed, will be suitable.

B.4.2: The Computer-Monochromator Interface

There are two opposing directions in which the interface hardware can be developed. The hardware can be designed to enable control by an unmodified standard microcomputer of any of a broad range of types. A product of this design philosophy might be a hardware interface (perhaps with its own microprocessor) connecting the

various monochromator system components to, say, a standard serial port. This would allow the use of any computer with a serial port as the control computer, including the capability to change control computers readily. An interface design such as this can involve moderately complex hardware.

Alternately, the interface hardware can be designed for maximum simplicity, using standard off-the-shelf components as much as possible. Thus, the interfacing might consist of installing a number of stepper motor controllers (as internal interface cards) in a microcomputer, along with an interface card to read the output from the photodetector. This approach obviously requires a dedicated microcomputer. The choice of microcomputer is also restricted, as suitable interface cards must be available.

Elements of both of these design philosophies were used in the development of the monochromator system/control computer interface. As the TTL controlled stepper motor drivers from the original monochromator system were available, an interface with TTL inputs and outputs and the capability to read the photodetector output would be sufficient.

A PC-14 Digital Input/Output Card was chosen as meeting these requirements. The PC-14 is an IBM-PC compatible interface card built using two 8255 Programmable Peripheral Interface (PPI) chips and an 8253 Counter/Timer circuit. It provides 48 programmable TTL I/O lines configured as six parallel ports and three counter/timers. The external connectors are two 40-pin dual row pin connectors. A ribbon cable was used to connect the PC-14 to a data and control distribution unit, used to distribute the output from the PC-14 card to the various stepper motor controllers, and including the amplifiers to convert the photodetector output to a TTL signal (with power provided by the PC-14 card). The complete control system is shown in figure B-5.

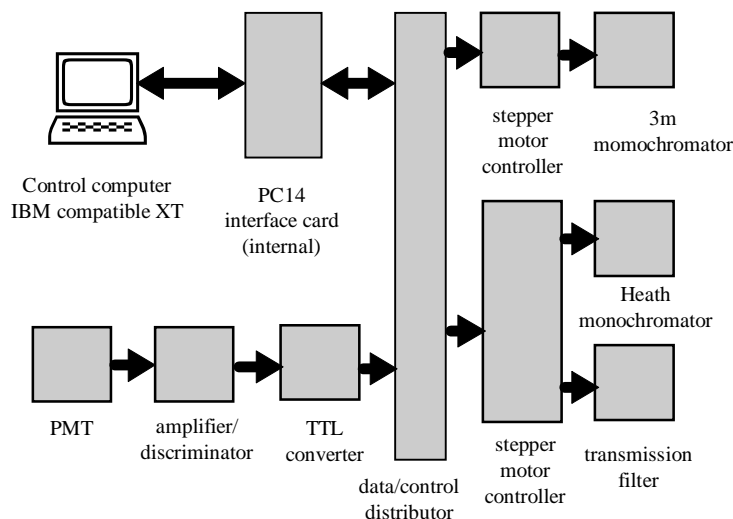


Figure B-5: PC-Monochromator Interface

The PC-14 card occupies twelve consecutive addresses on the PC I/O bus, with the different addresses being used to control the various functions of the PC-14 card.

B.4.3: The Control Software

The control software is an important component of the system. Without adequate software, a computer-controlled experiment is relatively useless. Well engineered software can greatly increase the ease of use and can generally improve the utility of the system. Appropriate care should therefore be paid to the development of suitable software.

The software must allow control of the basic monochromator functions, such as setting the wavelength, counting the output from the photomultiplier, and so on. More complex functions, such as scanning a section of the spectrum, are a combination of such simple operations. Ideally, all common actions can be performed by executing a single command. The software should also be designed so that the system can run unattended for long periods of time and perform multiple tasks in this time. This requires a degree of pre-programmability. Data processing software can also be included along with the experiment control software.

The software can either be a menu based system, readily allowing for interactive guidance for new or occasional users, who often prefer such systems, or a

simpler command line system. As the operating system used on the control microcomputer was MS-DOS 6.2, both could be readily developed.

Care must be taken to ensure that the period of time over which the photodetector output is counted is accurately known. On an IBM-PC compatible system, the shortest time intervals are those measured by the 18.2 Hz hardware timer interrupt (interrupt 8H). As a result, the shortest time period that can be accurately measured is 55 ms. Thus, it is convenient if 55 ms is used as a basic time unit, and counting times and pauses are measured in units of 55 ms. This is a convenient time unit to use for counting, as it is too short for the photomultiplier output to cause the counter to overflow, and is long enough to give a reasonable number of counts for a wide range of intensities. If a longer counting time is desired, a number of 55 ms counts can be made and combined.

The software used includes both a menu driven control interface, and a DOS command line control interface. A command line control command consists of:

command parameter1 parameter2 parameter3

The basic commands include those to move the system to a particular wavelength, report the current wavelength, *etc.* For example,

jump 6000

will set the system to a wavelength of 6000Å, and

where

would then give as output:

wavelength 6000.00 Angstroms

Position 298633 steps

Heath 60000 steps

Filter 4 steps.

A great deal of versatility can be built into such a system, including the use of various optional parameters. More complex commands can also be used. For example, a region of the spectrum can be scanned and the data saved by

scan 6000 6005 10 fe6002.

In this case, the counting time for each data point would be ten time units (of 55 ms) and the data would be saved in a file "fe6002.raw".

As each control command is a single MS-DOS command line, a sequence of such commands can be combined in an MS-DOS batch file (.BAT). This provides a high degree of programmability for the system.

The output is stored as an ASCII text file, with a header at the start of the file containing details on the file contents, such the time and date of data acquisition. The data can then be processed by the various data processing and display functions available as part of the monochromator control software package, or can be accessed by other software. For convenience, a MATLAB/monochromator data file converter was written.

B.5: Calibration of Monochromator System

A system used for emission measurements must be calibrated for its spectral response. This is necessary if relative intensities of lines at different wavelengths are desired. As the likely use of the intensity ratios is to find an unknown oscillator strength from a known value, using equation (A-23),

$$g_i f_{ij} = g_0 f_0 \frac{I_{ij} \lambda_{ij}^2}{I_0 \lambda_0^2} \quad (\text{B-3})$$

where the intensities are measured in photons per unit time, it is sufficient to find the system output per input photon as a function of wavelength.

The simplest calibration method is to use a source with a known intensity-wavelength function, and to measure the output from this source using the system. The source can either be a line source, with well known line intensities (or at least well known line intensity ratios) and with lines available at suitable wavelengths, or a continuum source.

The source used to calibrate the system was an SR 76 tungsten ribbon filament incandescent lamp with a fused silica plane window. The lamp was operated with a current of 35A, which gives a maximum emission wavelength of 1.05μ . The absolute spectral radiance of the lamp was measured by CSIRO.³ Such a source can be used to

³CSIRO Division of Applied Physics "Report on One Tungsten-Filament Lamp" Commonwealth Scientific and Industrial Research Organisation (1982).

determine the absolute response of a spectroscopic system, or can be used to find the relative spectral response. The relative spectral response can be determined more accurately, and is sufficient when measuring line intensity ratios.

B.5.1: Spectral Response of System

The spectral response of the system can be determined by measuring the system output for known inputs at suitable wavelength points. The SR 76 standard lamp described above was the source used. Measurements were made at 100Å intervals in the wavelength range 3000Å to 7300Å. The results (converted to number of photons input per unit detector response) are shown in figure B-6.

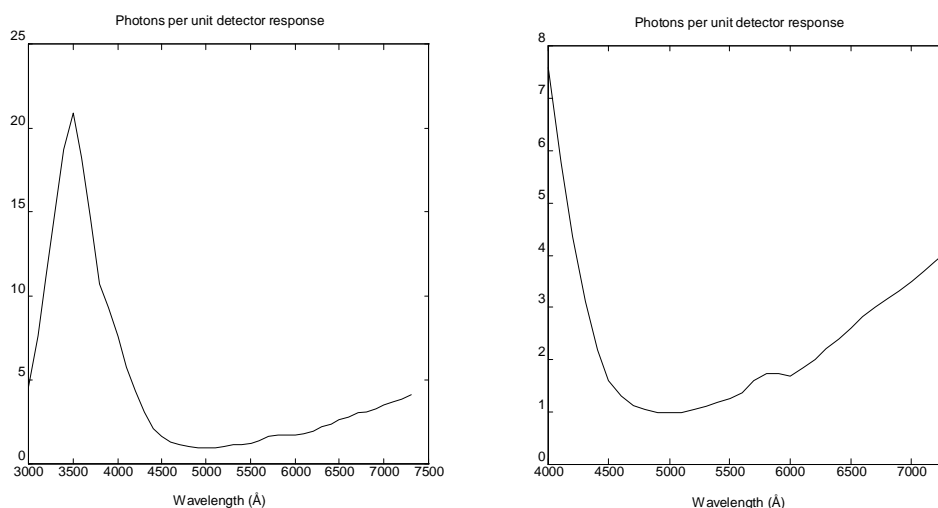


Figure B-6: Calibration Curve for Monochromator

The system response for wavelength points other than those measured can be found through interpolation from the measured values. The peak response of the system is at 5000Å. The sensitivity of the monochromator system in the visible spectrum is quite good, but is somewhat worse in the ultraviolet spectrum. Spectral lines of interest in the visible solar spectrum obviously will not be in the ultraviolet spectrum, but reference lines with known *gf*-values and sharing a common upper level may be. The increased uncertainty in calibration in the ultraviolet can thus be a problem.

Generally, it is desirable to find line intensity ratios for lines close together in wavelength. Calibration errors are then minimised. If lines are far apart in wavelength, the calibrations for the spectral response of the system is likely to be the greatest source of error. For lines in the visible spectrum, the error in the intensity ratio due to the calibration is estimated to be less than 5%. If lines are close in wavelength, this error will be much smaller. Measurements involving ultraviolet lines will have larger errors, and are therefore less desirable.

B.6: Measurement of Line Intensity Ratios

The procedure of measuring line intensities is fairly straightforward. The intensities of the desired lines are measured by the system for a time period long enough to give the required photometric accuracy. Lines from a common upper level must be measured with identical conditions in the hollow cathode source to ensure identical upper level populations. Either pairs of lines can be measured in order to determine an unknown oscillator strength from a known value for the reference line, or all (important) lines from a given level can be measured in order to find branching ratios and oscillator strengths from the lifetime of the upper level.

If the occurrence of self-absorption is suspected, multiple measurements under different source conditions can be made as a test. The first, and simplest, step is to examine the line profile for any obvious effects of self-absorption (see figure A-1).

B.6.1: Line Intensity Measurements

Some examples of line intensity measurements made using the system described here are shown in figure B-7.

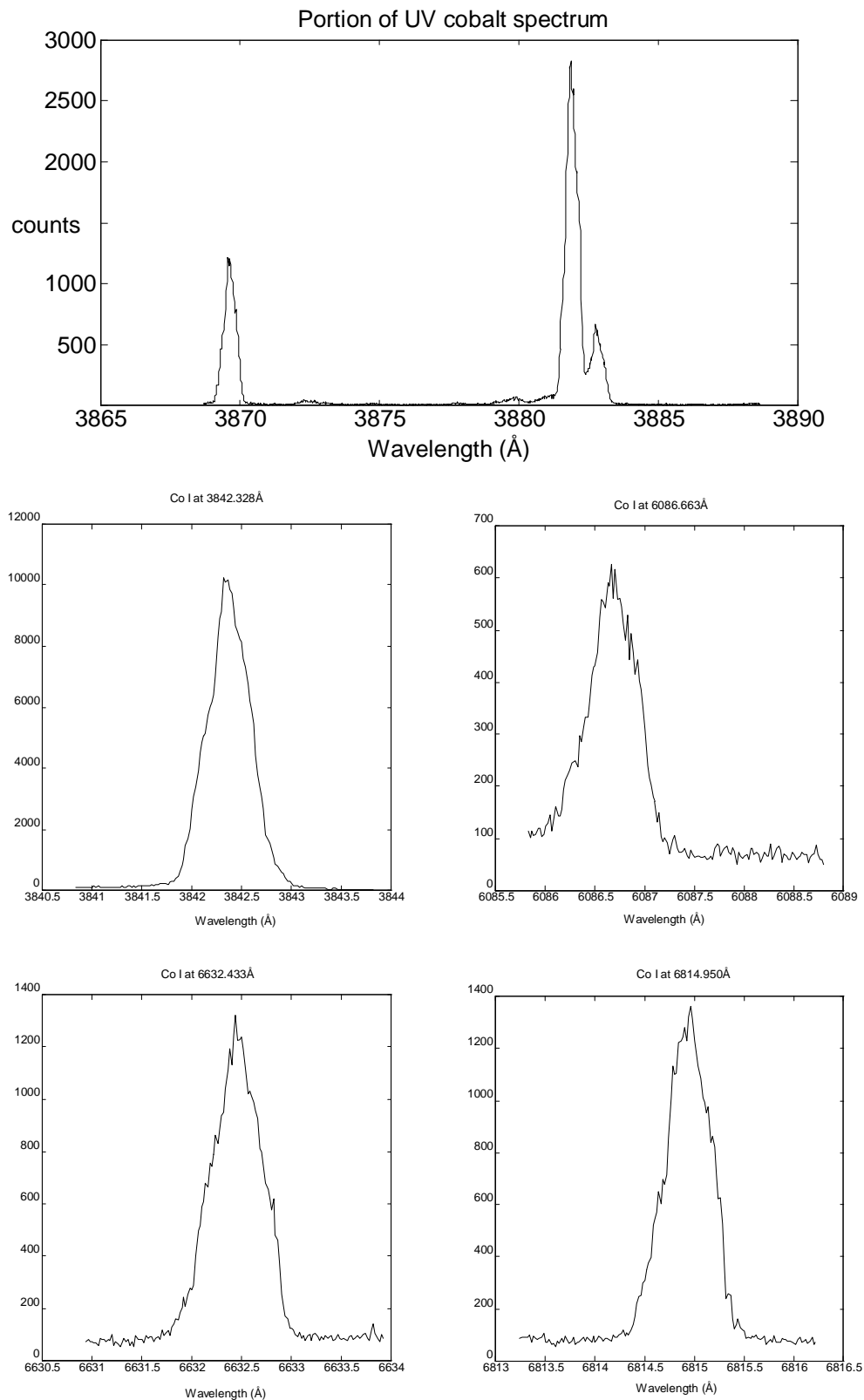


Figure B-7: Line Intensity Measurements

The approximately triangular profile of the emission lines shown in figure B-7 is due to the width ($\approx 80\mu$) and alignment of the exit slit of the 3m monochromator.

The importance of having a low level of background noise can be seen from the weak line measurements.

B.7: Oscillator Strengths

Oscillator strengths can be found from known gf -values by using the line intensity ratio. From equation (A-23),

$$g_i f_{ij} = g_0 f_0 \frac{I_{ij} \lambda_{ij}^2}{I_0 \lambda_0^2}. \quad (\text{B-4})$$

If the lifetime of the upper level is known, the branching ratio, defined by equation (A-22)

$$R_{ij} = \frac{I_{ij}}{\sum_k I_{ik}} \quad (\text{B-5})$$

can be used to find the oscillator strength as the Einstein spontaneous emission coefficient for a transition is given by

$$A_{ij} = \frac{R_{ij}}{T_i} \quad (\text{B-6})$$

where T_i is the lifetime of the upper level.

If the lines involved are close together in wavelength, the greatest error is likely to be due to uncertainties in the reference line oscillator strength or the level lifetime. If the lines are separated in wavelength, the system calibration is likely to be the greatest source of error. With the spectroscopic system described here, it is possible to measure oscillator strengths to within 7% (or better for some lines).