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Computer-controlled Optical Spectrometer

Abstract: Hardware developed to implement the computer control of a single-beam monochromator operating under a time-sharing system is described. A stepping motor and associated circuitry yield very precise wavelength positioning in an open loop configuration and with a minimum of computer use. The circuits used to position and step the wavelength are described in detail.

Introduction

In this paper we describe the hardware used in a computer-controlled single-beam optical spectrometer. An IBM 1800 computer operating under the time-sharing system of H. M. Gladney[1] controls the spectrometer performing most of the usual functions including sweeping the wavelength, collecting data from sample and reference beam, and finally treating and displaying the data. The use of time sharing allows us the luxury of a sophisticated computer balanced by reasonable expense. However, to be compatible with time-sharing, a particular experiment must not place undue demands on the computer. Our hardware design satisfies this compatibility requirement by operating in an open-loop configuration and also by *not* working in a demand/response mode.

Two major and immediate improvements in our optical spectrometer due to automation can be mentioned. The first is the ease with which sample and reference data are handled and the second is the ease with which time averaging techniques (catting) can be used. In a research laboratory, it is often advantageous to have the flexibility of a single-beam instrument over the more routinely operated double-beam instrument. In general, it is easier to design optical experiments utilizing external parameters such as stress, temperature, electric and magnetic fields around a single-beam instrument. However, use of a single-beam instrument in absorption spectroscopy requires that the system response, i.e., a reference signal, be generated and divided out of the sample plus reference signal. This division of sample and reference beam can be slow and tedious when done by hand but, of course, is a trivial calculation for a computer and a recognizable sample response can be available almost immediately after the sweep is concluded.

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The efficacy of time-averaging techniques has been amply demonstrated[2,3] and is especially well suited to a computer-controlled experiment. The computer can repeat an experiment any number of times, terminate the time averaging on some condition, e.g., helium level in a dewar or signal-to-noise ratio of an expected signal, and switch to another experiment, all done unattended at midnight as well as midday. A persuasive example of time averaging performed on our automated spectrometer is shown in Fig. 1, which gives the so-called *B*-line absorption of Mn^{4+} in $KTaO_3$. The upper plot is a single scan and shows one absorption line with a possible second line (signal/noise ratio $\simeq$ 1) adjacent to it. The lower plot is the time average plot of 25 scans and shows this second line well enough to determine the usual amplitude, width, and line shape parameters. The 25-scan, time-averaged plot represents no more effort to the experimenter than does the single scan, the difference being, of course, the longer experiment time for time averaging.

Another advantage of computer use in spectroscopy lies in the handling and storing of data. Results can be stored on disk or tape and be retrieved later for further mathematical analysis or for comparison with another spectrum. Also, we can envision exchange of data via tapes or disks and, to complete the picture, central data banks with general spectral information readily available over telephone lines. This last idea would apply to analytical measurements such as x-ray and infrared data more than optical spectroscopy.

As indicated above, this paper deals almost entirely with the hardware aspect of our automated spectrometer. Simply stated, the main purpose of the hardware is to control the drive shaft of the diffraction grating in a monochromator. This control divides into two functions: to position the diffraction grating at a starting wavelength and

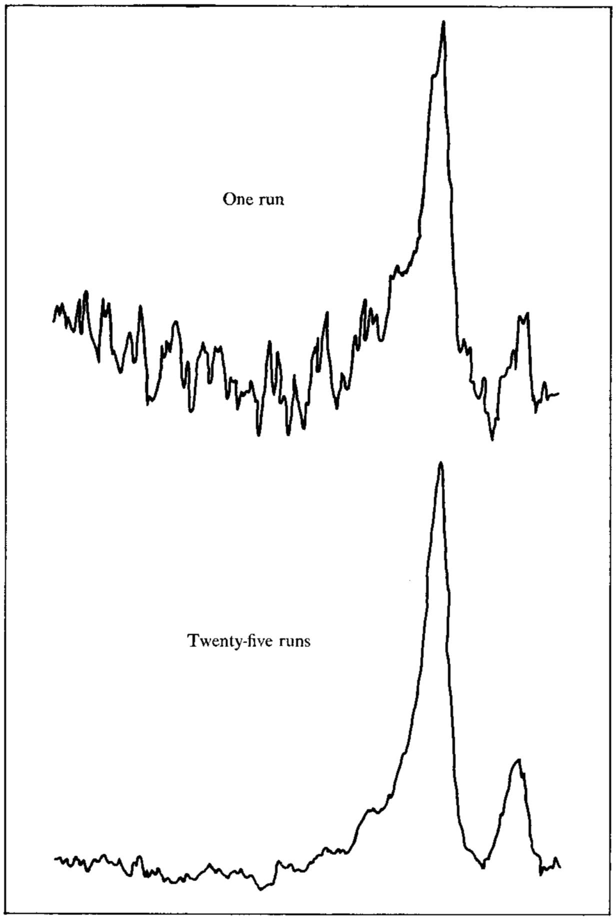


Figure 1 Example of time averaging.

to turn the grating or equivalently to step the monochromator wavelength for a preset number of Angstroms. Although we apply the hardware to our monochromator it will be apparent that it is applicable to any situation where shaft position and rotation is controlled.

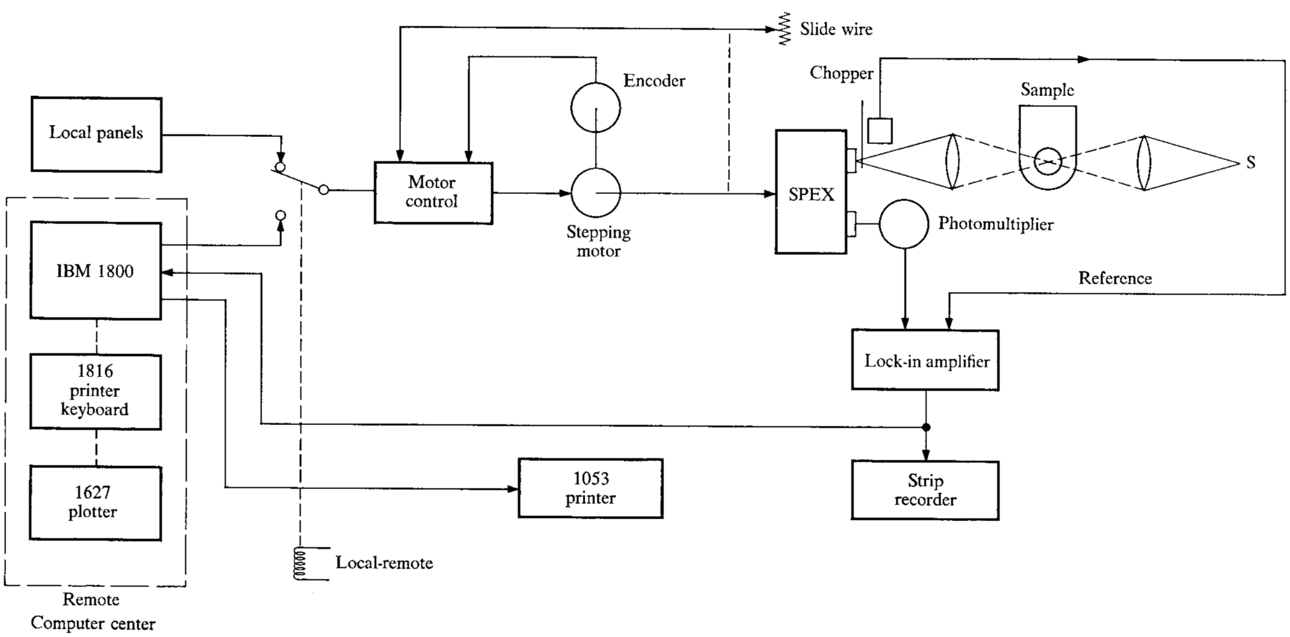
An IBM Research Report[4] describes the software used to control our spectrometer. We refer the reader to Grant[5] for a more extensive discussion of software used to control an optical spectrometer, and to Johnson et al.[6] for interface design.

The following section describes our spectrometer system and the subsequent section the details of the hardware. An Appendix gives the actual circuits used.

The spectrometer

Figure 2 is a block diagram of our system. The section within broken lines is located approximately 300 ft from the experiment. Energy from a source (tungsten or mercury-xenon lamp) passes through the quartz tail of a helium dewar containing a sample. The light coming from the sample is chopped at 90 Hz and focused on the entrance slits of the Spex grating monochromator. Light of the selected wavelength is passed through the monochromator and detected by the photomultiplier. The photomultiplier signal is phase detected in the lock-in amplifier and the output is recorded on the strip chart and also sent to the computer as an analog signal. This part of the experiment is unchanged from pre-computer systems except that the analog voltage is now sent to the computer.

Figure 2 Optical spectrometer system.



The major hardware changes occur in the grating positioning system. Originally the diffraction grating was positioned by a motor internal to the monochromator. In the computerized design a 200 step/revolution stepping motor is attached directly to the grating drive shaft. One revolution of the drive shaft is 50 Å; thus a single step is $\frac{1}{4}$ Å. Attached to the motor shaft is a one-position shaft encoder designed to resolve one step or 1.8° (see Fig. 3). The stepping motor is driven at approximately 50 Å/sec using a SLO-SYN translator Module Type STH 1800V.* As mentioned, the hardware performs two functions, setting the starting wavelength and stepping the wavelength a prescribed number of angstroms for a prescribed number of data points.

The starting wavelength can be chosen every 50 Å throughout the useful monochromator range. As described below, this starting wavelength is precise to at least one step of the stepping motor ($\frac{1}{4}$ Å). If a starting wavelength between 50 Å positions is desired, it is a simple matter to move to the nearest set position then add the difference through one step of the stepping sequence described below.

The considerable precision of the starting wavelength is obtained by combining an analog device and a digital device. The monochromator is equipped with a 1542 Wavelength Analog takeoff§, a 0.1 percent (approx. 15 Å) precision slidewire potentiometer, with a wiper which moves with the monochromator sine-bar drive.† The wiper voltage is proportional to wavelength and is used to bring the wavelength drive to within one revolution (50 Å) of the set wavelength. When the drive is within one revolution of the set wavelength, the analog signal no longer is operative in positioning the wavelength. The stepping motor continues to step in the same direction until the one-position optical encoder signals a 50 Å position and the stepping motor is stopped. The circuit details will be described but we wish to emphasize here that it is the combination of a moderately accurate analog signal and a one-position optical encoder that yields a very precise wavelength set.

We now describe the stepping operation. For this paper the term "step" is used to denote the interval between data points and not a single step of the stepping motor. The minimum "step" is one step of the motor, or $\frac{1}{4}$ Å, and the programmed "step" is some multiple of this minimum. For example, if a data point spacing of 2 Å is desired, the "step" is eight steps of the motor. The "burst counter" is a circuit which counts the oscillator pulses sent to the stepping motor and opens a relay when it has accumulated a count (of $\frac{1}{4}$ Å motor steps) equal to the programmed "step." For a single "step" the translator module oscillator is connected to the motor and to the burst counter on command from the computer. The motor steps until the burst counter relay opens and interrupts the oscillator pulses going to the motor. At present the counter is an eight-bit binary counter allowing a maximum step of 63-$\frac{3}{4}$ Å.

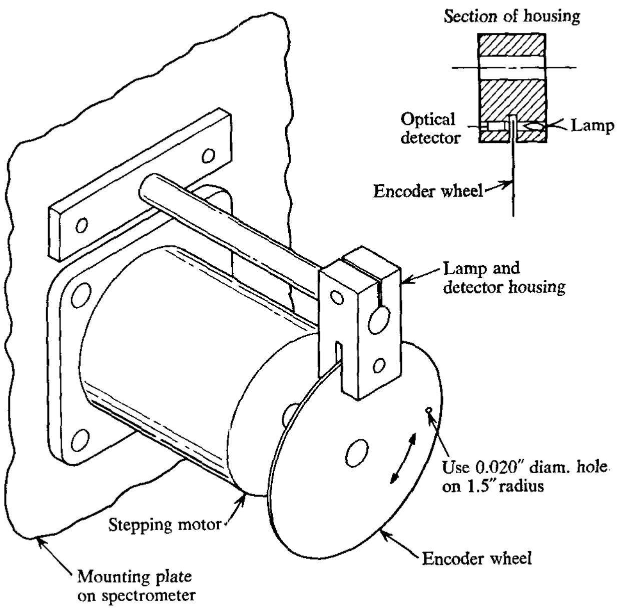


Figure 3 Stepping motor and one-position shaft encoder.

The full stepping cycle consists of reading the signal from the P.A.R., stepping the grating the required number of Angstroms and waiting a time characteristic of the integrating time of the phase detector. This process is repeated for the number of data points requested. The above two cycles, setting the wavelength and stepping, are repeated but with sample replaced by a reference cell. Finally the ratio of the sample and reference runs is plotted on a Calcomp plotting. A time averaging operation is accomplished by repeating the runs the desired number of times, adding the results and plotting the average.

Figure 4 shows the laboratory control panel. Section I contains controls for local operation of the monochromator including speed (frequency) control, direction control and run vs single-step control. The mid-area of the rack contains the computer input with the double row of panel indicators. Two 16-bit contact operate words are used to control the experiment. The lower area of the control panel has local controls which parallel the computer controls, a useful feature when testing the equipment.

An experiment is initiated from the laboratory using the interrupt facility of the computer. The called interrupt program reads the input data as contents of panel switches

* Superior Electric Company, Bristol, Conn.

§ Spex Industries, Inc., Edison, N. J.

† An external multiturn potentiometer may be used.

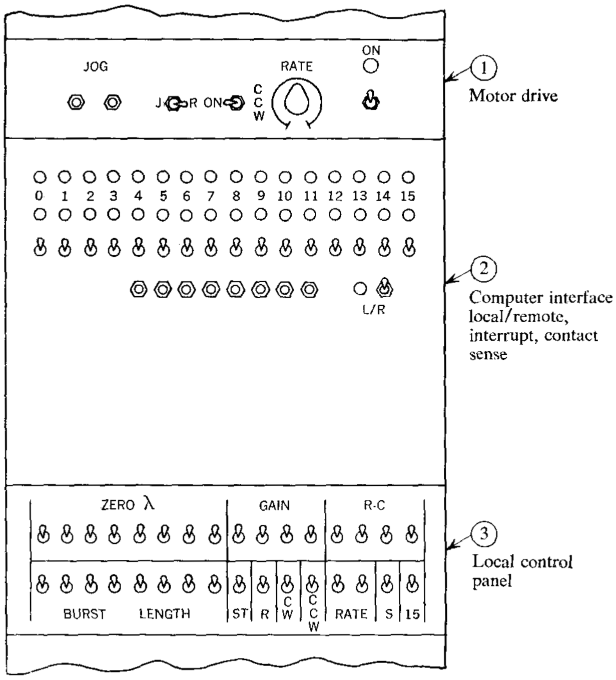


Figure 4 Laboratory control panel.

and prints out the initializing data on a 1053 Printer in the laboratory. This printout serves as a validity check on input data and also as a record. If the input data is satisfactory, the interrupt program places the "run" program into the 1800 process queue. The run program, executed after approximately one minute, moves the monochromator to the starting wavelength and commences the stepping operation.

Hardware details

We now describe the hardware system in block diagram form and give the actual circuit diagrams in the Appendices. Figure 5 shows the interconnection of the wavelength set circuitry, the stepping circuitry and the Translator module. The module contains a pulse oscillator and the logic required to convert a single pulse into the pulse train which steps the motor. As outlined schematically in Fig. 5 the stepping circuitry and the wavelength set circuitry have very similar functions, that is, they direct the oscillator pulses to the motor logic to step the motor in the desired direction. The wavelength set circuitry interrupts the pulses when the set position is reached and the stepping circuitry interrupts when it has accumulated the programmed number of pulses.

The stepping circuitry may be used to provide reset by programming the return step required to reach the starting wavelength. For scans of less than 50 Å we do use the stepping circuitry to provide reset. However, it is important to note that any stepping motor error is cumulative if stepping circuitry is used for reset whereas it affects only one scan of a time averaging operation when wavelength set circuitry is used. This is so because the wavelength set circuitry uses a fiducial mark, the optical encoder, while the stepping circuitry simply counts.

• *Wavelength set*

Figure 6 gives the wavelength set diagram. The reference voltage circuit develops a voltage difference proportional to the difference between the set point and the wiper or grating position. The amplified difference voltage selects the direction of the motor. Upon a reset command, the motor reset circuit connects the oscillator and motor and also energizes a latching circuit involving the one-position shaft encoder. The motor commences to step the grating toward the set point, decreasing the difference voltage. When the difference voltage falls below a certain voltage (equivalent to approximately 25 Å or one-half revolution) the directional relay (see Appendix A) would open but does not because of latching action of the encoder circuit. The next 50 Å position is signalled by an encoder pulse which unlatches the directional relay, stopping the motor.

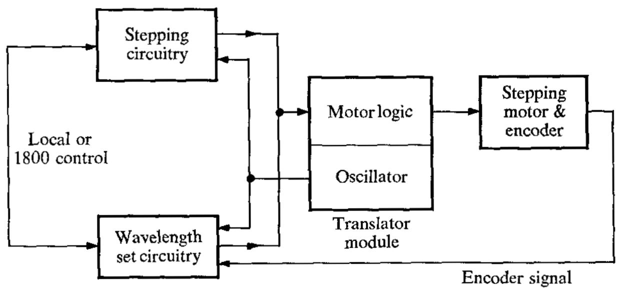
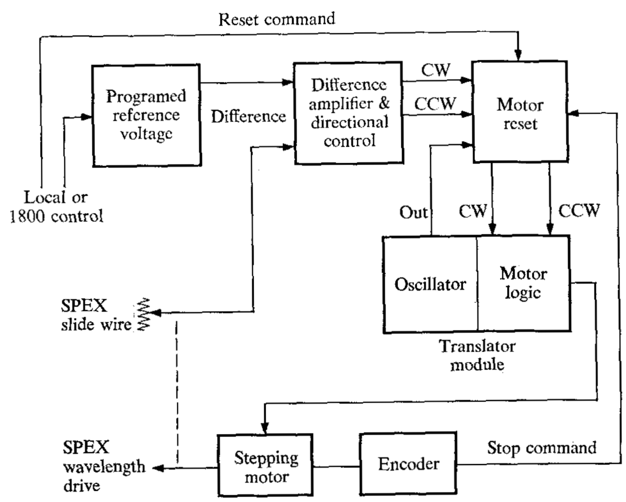


Figure 5 Hardware system block diagram.

Figure 6 Wavelength set block diagram.



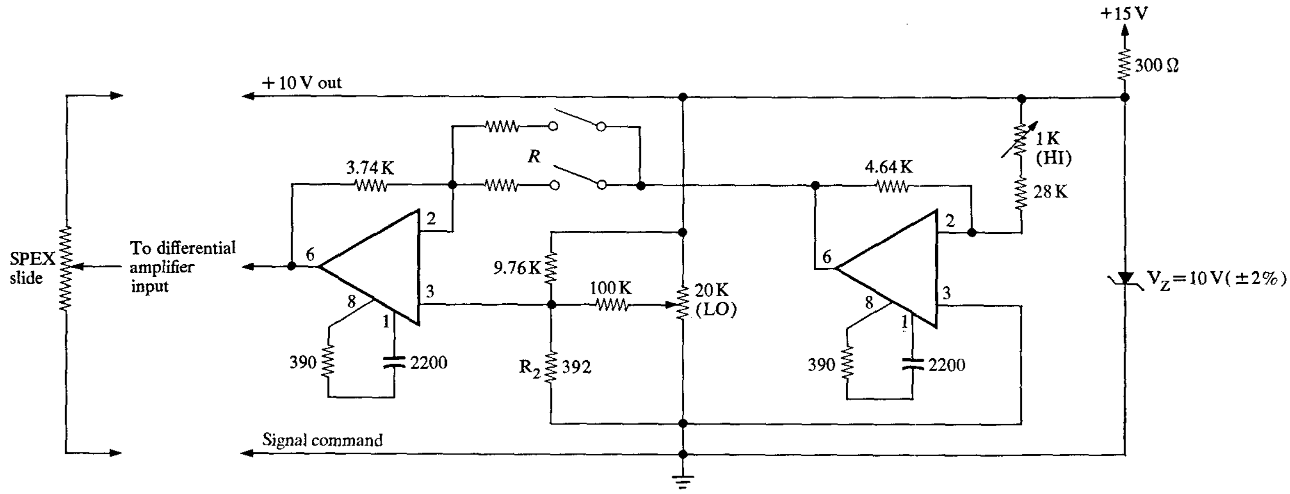


Figure 7 Programmed reference (*R* is programmed with an 8-bit relay network).

A few general comments on the wavelength set circuitry may be useful. The purpose of the circuit is to position the monochromator grating with high precision and with mininum use of the computer. In our design the computer sets the relays in the reference voltage circuit and operates the reset command relay. The experiment is then free of the computer and the wavelength is set without the use of a closed loop system and without actually determining the initial grating position. The system allows approximately one minute for the grating to reach the set wavelength before commencing a sweep.

• *Stepping sequence*

Figure 10 gives the circuit diagram for the burst counter and associated circuitry which make up the stepping circuitry of Fig. 5. Details are described in Appendix B. Here we give a brief operational description.

Oscillator pulses from the translator module, Fig. 5, are not transmitted to the motor logic until the computer sends a step command. This step command allows the next oscillator pulse to close relays which connect the oscillator to the burst counter and the motor. The second oscillator pulse then is counted and also steps the motor. Using the first oscillator pulse after the step command rather than the step command itself, to connect oscillator to motor and counter, guarantees that they are synchronized and eliminates the problem of responding, in either circuit, to a fraction of a pulse.

The step command for stepping operation is sent by the computer in time intervals calculated from the time constant of the lock-in amplifier and the speed of the motor. Usually points are read every few seconds. We mention but do not describe other controls which complete the two 16-bit words sent by the computer to the experiment. Four bits are reserved for gain control, two bits for time constant, two bits for motor speed control, two bits for direction of step, one bit for sample change and the remaining three bits for auxiliary functions not yet specified.

Discussion

The discussion divides into comments on the hardware for the shaft positioning system and comments on our approach to spectrometer automation since the value of one is more or less independent of the other.

Concerning the hardware, our experience indicates that the circuits used are quite reliable and not overly critical. The resistor chain, Fig. 7, and the internal resistor (or external potentiometer) do require 0.1 percent precision and linearity. This precision is determined by our requirement that the analog circuit differentiate between two 50 Å points in a total of 15,000 Å or, as a shaft position requirement, one turn in three hundred. Shaft positioning circuits in a situation with fewer total turns would need proportionally lower precision. An important aspect in a time-sharing system is how much and how critical is the demand on the computer. In our system the computer commands either reset or step and is then free of the experiment since both operations are performed in an open loop fashion. Also, the system does not operate in a demand/response mode. The experiment can wait at a wavelength until the computer is ready to accept the datum. In summary, the hardware described is precise, reasonably easy to build and places a minimum demand on a computer in a time-sharing system. Further, the hardware is not designed for a specific computer nor for a particular time-sharing system but is applicable where shaft rotation

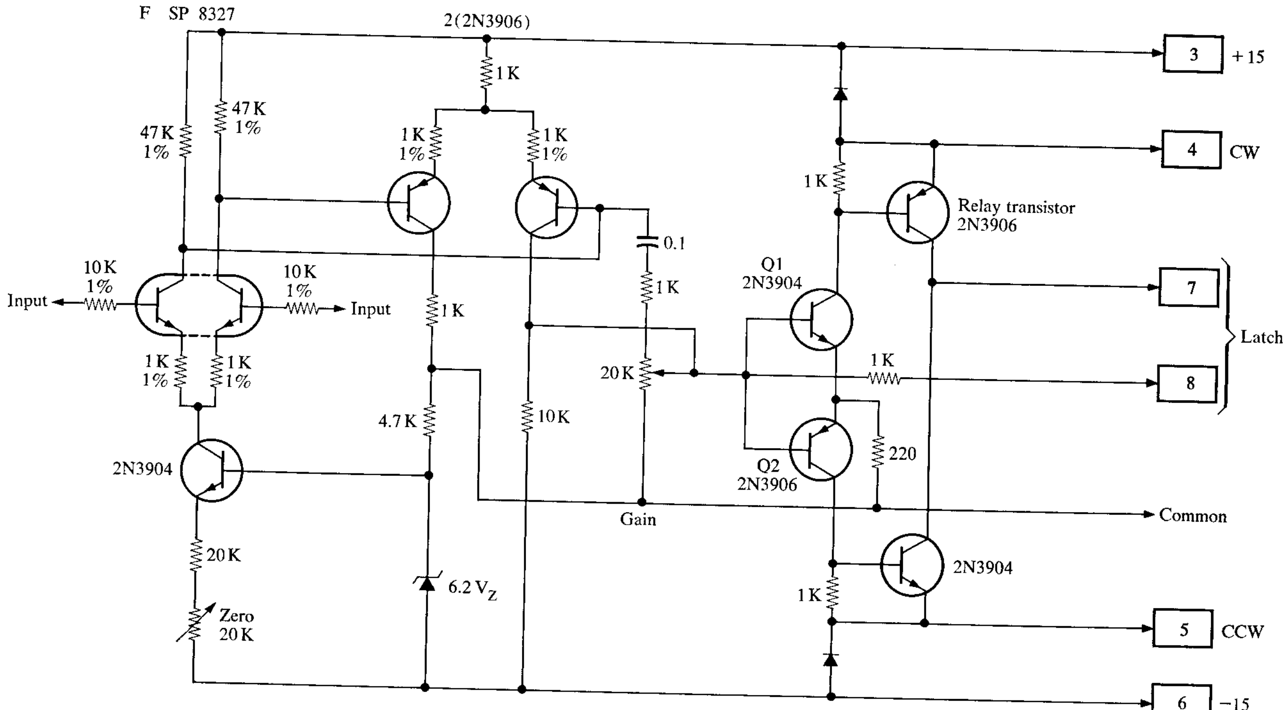
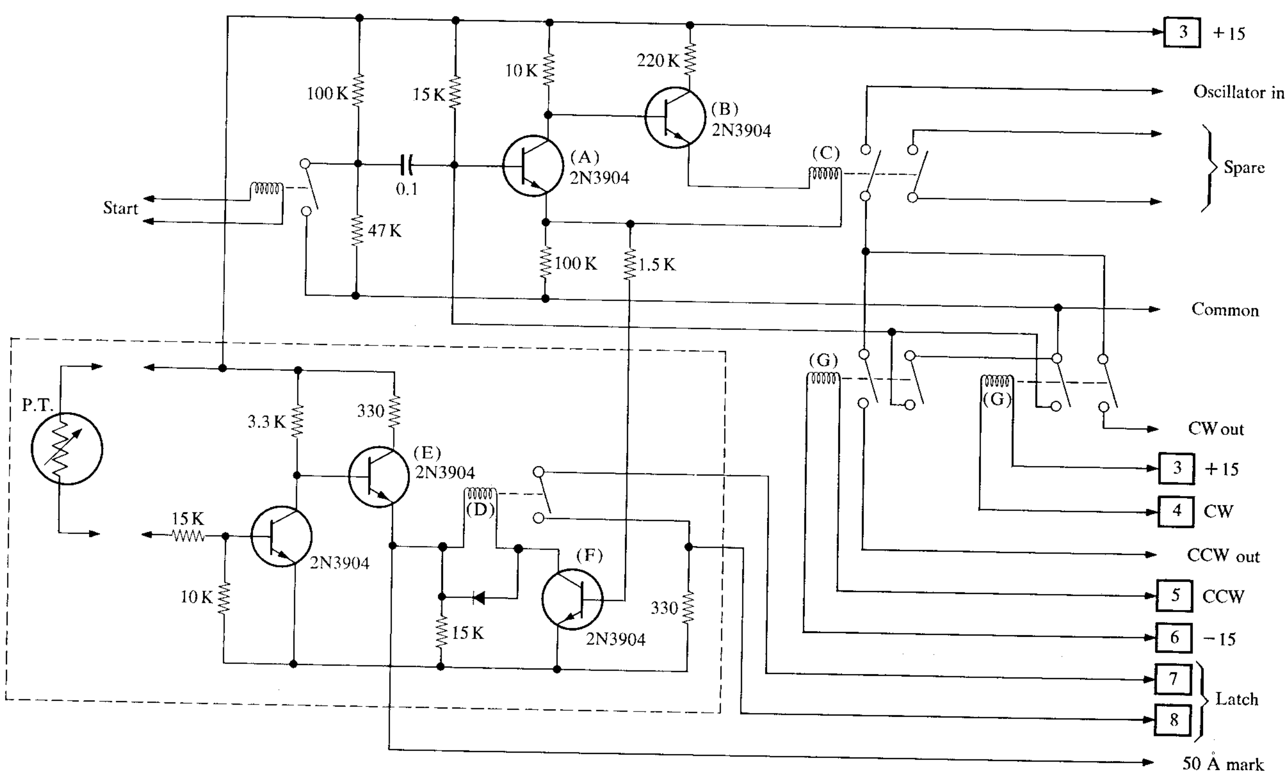


Figure 8 Difference amplifier.

Figure 9 Motor reset control.



is to be controlled by a computer.

A few comments concerning the over-all spectrometer design are appropriate. We send our data to the computer (a distance of 300 feet) as analog signals in an individually shielded twisted pair cable. The computer then performs the analog-to-digital conversion. Experiments in this lab[7] indicate that no appreciable noise is added to the analog signal with this arrangement. Another point of concern is the switching rate between sample and reference. Usually a scan takes a few minutes and therefore noise or drift with a few-minute period can affect the signal/noise ratio.[3] Measurements taken after suitable warm-up time on source and detector, show that such drift does not have a deleterious effect on our signal/noise ratio. Finally, we re-emphasize that the flexibility desirable in a research instrument is obtained using straightforward hardware and allowing the software programming to yield variety in experiments.

Appendix A—Wavelength set circuit

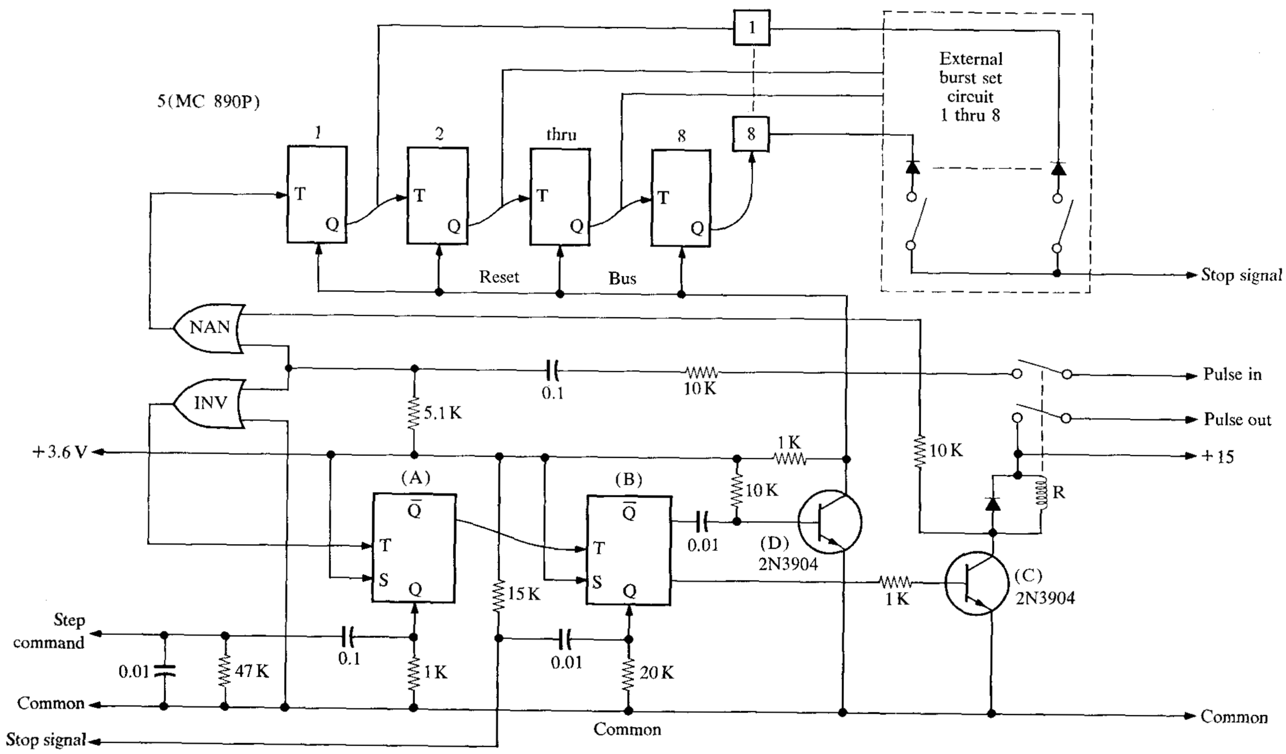
This section gives details of the reference voltage circuit, the difference amplifier and the motor reset circuit.

Figure 7 gives the circuit diagram of the programmed reference voltage. Two operational amplifiers are used to give a positive voltage proportional to the conductance of the parallel resistor net *R*. These eight resistors, of which two are shown, are chosen as $2^n R_o$ (R_o = 2K and n goes from 0 to 7) and programmed as one half of an computer contact operate word, i.e., 8 bits. The same voltage (10 volts) presented to the operational amplifier circuit appears across the slide wire, making the difference voltage ratio independent of the supply voltage. The 1K variable resistor adjusts the gain of the operational amplifier correcting the end effect on the high end of the slide wire and the voltage across R2 compensates for the end effect on the low end of the slide wire.

The difference voltage is fed to the difference amplifier, Fig. 8, and, after amplification, causes Transistor Q1 or Q2, depending on sign of voltage difference, to conduct. The conducting transistor biases its relay transistor into the conducting region which then selects the motor direction and also grounds the base of Transistor A of the motor reset control, Fig. 9. The numbers in the squares on the right side of Figs. 8 and 9 indicate connections between the difference amplifier and the motor reset control. To commence a wavelength set, the start relay of Fig. 9 is closed, biasing Transistor A off, which in turn biases Transistor B on, closing Relay C. Relay C completes the circuit between oscillator and motor which then steps at 50 Å/sec toward set point.

The part of the motor reset control outlined in broken line is the latching circuit. To close Relay D of the latching

Figure 10 Burst counter.



circuit, both Transistors E and F must be conducting. Transistor E conducts when the photocell is dark (high resistance). During the wavelength set cycle Relay D is closed except for 50 Å points when the optical encoder allows light onto photocell and Relay D opens briefly. As the motor steps toward the set point, the amplified difference voltage falls below the base voltage needed to keep Transistor Q1 or Q2 of Fig. 8, conducting. This crossing point is adjusted by the gain control to occur for a difference voltage equivalent to less than one revolution. (Approximately 15 mV difference at input 1, 2). Reaching this critical voltage does not turn off Transistor Q1 or Q2 because the latching relay directs collector current through the 1K resistor to supply base voltage. At the next 50 Å mark from the photocell the latching relay opens and the base voltage of Transistor Q1 or Q2 falls below the conducting region. The relay transistor is, in turn, biased off, opening CW (or CCW) relay. Relay G on motor reset circuit opens raising base voltage of Transistor A and through B opens Relay C. The grating is now at the prescribed starting wavelength and the wavelength set circuitry is in its initial state.

Appendix B—Stepping circuit

Figure 10 gives the diagram for the burst counter and associated circuitry which make up the stepping circuitry of Fig. 5. In this description a knowledge of logic elements is assumed. The negative oscillator pulses (−10V, 50 msec) are inverted and sent to flip-flop A. The trailing edge of the pulse (negative going) at T of flip-flop A is steered by S voltage to make the state of $\bar{Q}$ a 0. However, the initial state of $\bar{Q}$ is 0 and the pulses at T do not change the state of flip-flop A. Upon the step command, flip-flop A is reset and $\bar{Q}$ goes to 1. The next oscillator pulse at T change $\bar{Q}$ to 0 and pulses T of flip-flop B. $\bar{Q}$ of B goes from 1 to 0, dropping base of Transistor D, which raises the reset bus of the burst counter. Now the counter is zeroed. $\bar{Q}$ of B goes from 0 to 1 which causes Transistor C to conduct closing Relay R and also lowering voltage to NAN circuit. The next pulse goes to stepping motor through Relay R and also goes to burst counter through the NAN circuit. The NAN circuit gives a positive voltage out when both inputs and effectively negative.

The stepping sequence continues until the burst counter accumulates the number programmed in the relays. This match of counter and relay contents raises the voltage at the reset point of flip-flop B through the stop signal. When B is reset Q goes to 0 and Transistor C stops conducting. Relay R opens stopping the motor and the voltage to NAN goes positive, stopping pulses to the counter.

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