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To the Graduate Council:

I am submitting herewith a thesis written by John Alva Herndon entitled "Design and Construction of a Vacuum-Grating Spectrograph for the Infrared". I recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Physics.

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DESIGN AND CONSTRUCTION OF A
VACUUM-GRATING SPECTROGRAPH
FOR THE INFRARED

A THESIS

Submitted to
The Graduate Council
of
The University of Tennessee
in
Partial Fulfillment of the Requirements
for the degree of
Doctor of Philosophy

by

John Alva Herndon

December 1957

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CHAPTER I

INTRODUCTION

The Need for a New Spectrograph

The Department of Physics of the University of Tennessee has for a number of years been one of the leading institutions in the United States in the field of high resolution infrared spectroscopy. Just prior to World War II the Department built a high resolution prism-grating spectrograph which was designed to utilize the best diffraction gratings and infrared detectors then available. Since that time larger and better quality gratings have become available, and new and improved infrared detectors have been developed, thus making it possible to obtain higher resolving power. Also, methods of frequency determination have been improved and simplified by the use of Fabry-Perot calibrating systems.

As these improvements became available the original instrument was modified to utilize them. However, the optics of the instrument were not large enough to accomodate the full area of the larger gratings and the mechanical features of the instrument made it difficult to utilize the full potentialities of the new detecting systems. These factors limited the resolving power of the instrument.

In certain parts of the infrared one is faced with the problem of removing water vapor and carbon dioxide from the optical path of the spectrograph because these molecules strongly absorb certain parts of the spectrum, thus hiding the absorption spectra due to samples

under investigation. It is thus necessary to "dry" these unwanted molecules from the spectrograph. This can be done to a large degree with the improved chemical drying techniques which have been developed in the last few years, but these techniques are still not good enough to remove the last traces of these absorbers. And these last traces must be removed if one is to make accurate intensity and line shape measurements. The best known method for removing these absorbing molecules is to enclose the instrument in a vacuum tank and pump all the air, water, and carbon dioxide from the system.

Enclosing the instrument in a vacuum also has the advantage that wave number measurements do not have to be corrected for the index of refraction of air as is necessary in the case of instruments which operate in air. Wave number values obtained with a vacuum instrument are thus more accurate than corrected values because the index of refraction of air in the infrared region is not precisely known.

Thus it was felt that if the University of Tennessee was to remain in a position of leadership in the infrared field it would be necessary to construct a vacuum-grating spectrograph which would take full advantage of the recent developments.

Type of Instrument to be Built

In the winter of 1954 funds were obtained by the Physics Department for the construction of such an instrument. It was immediately decided that a vacuum-grating spectrograph should be built which

would utilize the largest gratings available, the latest techniques in infrared detection, and a Fabry-Perot system for frequency determination.

A number of different optical arrangements could be used in such a spectrograph, and after considering these various arrangements at some length Dr. Alvin H. Nielsen decided that a Pfund type of optical system would afford the greatest simplicity, flexibility and accuracy for the type of research to be carried on.

Once the gross optical features were determined it was necessary to design a vacuum tank to house the instrument. No existing type of vacuum housing seemed to be completely satisfactory because of the cumbersomeness of the vacuum system covers which are normally lifted from the spectrograph by means of a chain fall. Therefore, a new type of vacuum tank was designed in which the cover of the system was mounted on wheels so that it could be rolled away from the spectrometer table.

After the vacuum tank and grating monochromator mirrors were ordered it was realized that the Pfund optical system could be modified by putting the entrance and exit slits close together and using one paraboloidal mirror as both collimating and condensing mirror. This modification would then reduce the size of the grating monochromator by reducing the number of mirrors in the system from four to two. This would make it possible to construct two of the modified Pfund grating monochromators with the same mirrors already ordered, and the vacuum tank would be large enough to house two complete spectrographs using this modified grating monochromator.

It was then decided that two spectrographs would be built. The first was to be a single pass instrument and the second a double pass instrument, i.e. in the first the radiation would be dispersed once by the grating before passing to the exit slit, and in the second the radiation would be dispersed once by the grating and then returned again to the grating to be dispersed a second time before passing to the exit slit. The reason for double passing the grating in this manner is that the resolving power of the instrument is doubled, provided that there is sufficient energy available to allow the slits to be narrowed. In the very near infrared there is frequently enough energy available to gain resolving power by double passing the grating; however, at longer wavelengths less energy is available and double passing is not advantageous.

The Problem

At the time the work was begun, it was proposed that the system be designed to be as automatic as possible without restricting the versatility and resolving power of the instruments. The plan was to construct parts for both single and double pass instruments in so far as the parts were alike, and then to complete the single pass instrument and determine its characteristics before completing the double pass unit.

With the gratings now available the theoretical resolution limit of the single pass instrument should range from 0.075 cm^{-1} to 0.030 cm^{-1} depending on the angle at which the grating is used. The gratings, however, are not perfect and will probably produce only

80 per cent of their theoretical resolving power. Thus it was expected that the single pass instrument would have a resolution limit of 0.095 to 0.037 cm^{-1} .

It was the aim of this work to carry out the above program, completing only the single pass instrument, with the hope of attaining the resolution limit stated above.

CHAPTER II

THEORETICAL CONSIDERATIONS

In designing a high resolution spectrograph for the infrared, one almost invariably chooses a reflection type diffraction grating as the principal dispersing element. It is thus necessary to know under what conditions the optimum resolving power can be obtained from such a grating spectrograph.

Let us assign a set of rectangular Cartesian axes to the grating G , Figure 1. G is a plane reflection grating with its rulings parallel

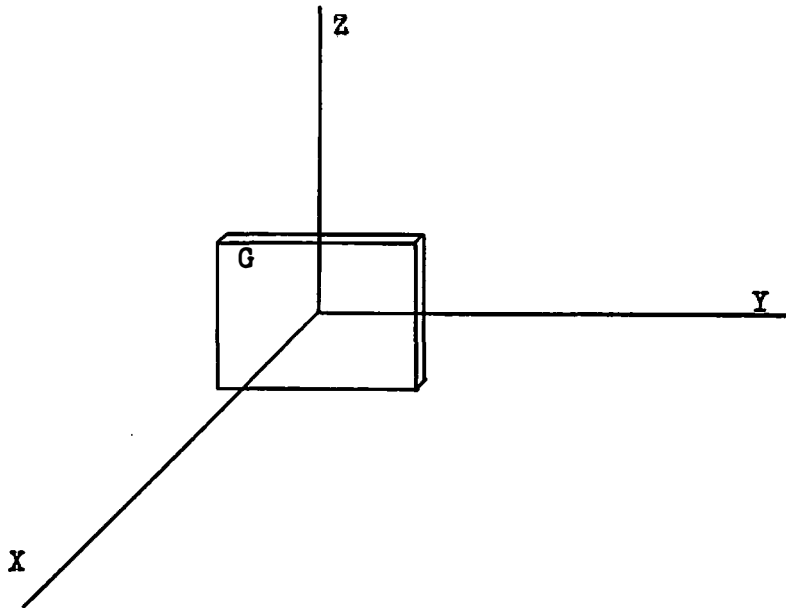


Figure 1. Grating axes

to the Z axis. The XYZ axes will be considered as fixed to the grating with the X axis normal to its center, the YZ plane being the plane of the grating face. We shall call the XZ plane the normal plane, and the XY

plane the equatorial plane.

If parallel white light is incident on the grating at an angle α to the normal plane and parallel to the equatorial plane, then parallel light of wavelength λ is observed at an angle β to the normal plane, Figure 2. The relationship between α , β and λ is given by the grating equation¹,

$$m\lambda = d(\sin \alpha - \sin \beta), \quad (\text{II},1)$$

where d is the grating spacing, and m is an integer called the order of

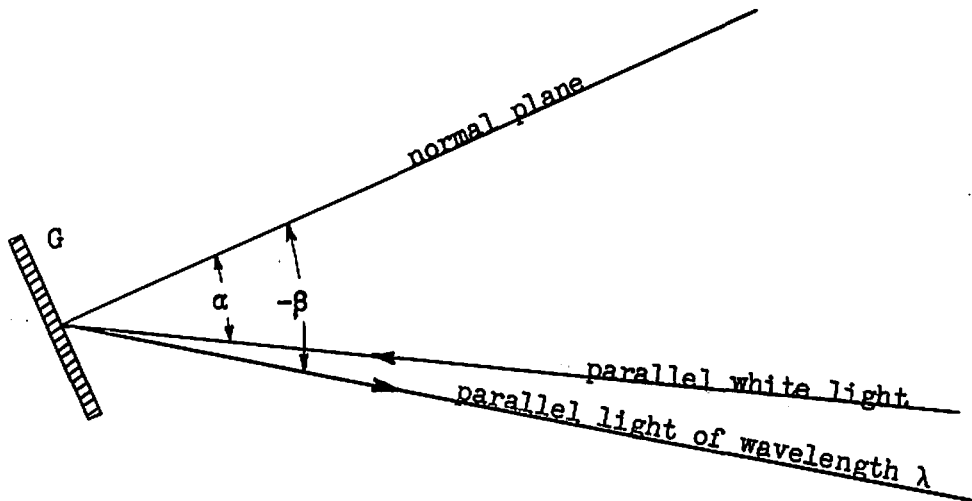


Figure 2. Grating angles

the spectral line or simply the order. It should be noted here that we have adopted the convention that β is negative if it is measured

¹F. A. Jenkins and H. E. White, Fundamentals of Optics (McGraw-Hill Book Company, Inc., New York, 1950), p. 327.

on the same side of the normal plane as α and positive if measured on the opposite side. For $\alpha = \beta$ the grating equation becomes $m\lambda = 0$. This means that m must vanish and λ can take on all values, so that at this value of β a direct reflection of the incident light is obtained. This direct reflection is called the central image.

It should also be noted that the grating equation as stated above holds only for light incident parallel to the equatorial plane of the grating. (See the section on Theory of Slit Curvature for a discussion of incident light making a small angle with the equatorial plane.)

Grating Equation for Fixed Slit Separation

Consider a modified Pfund type grating monochromator, Figure 3,

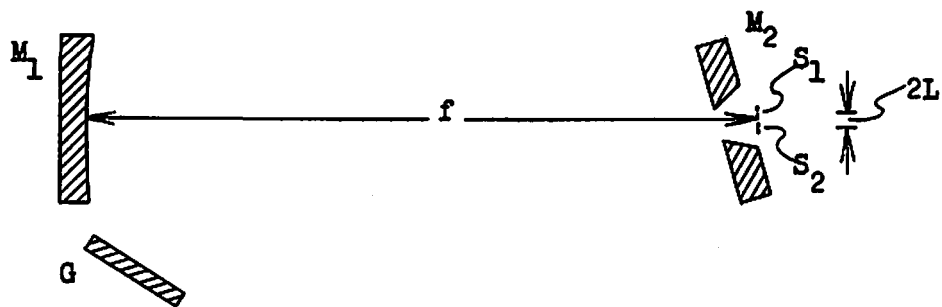


Figure 3. Pfund type grating monochromator

in which the entrance slit S_1 and exit slit S_2 are mounted behind the hole in the flat mirror M_2 . The slits are parallel to the Z axis of the grating G , and they are separated by a distance $2L$. The focal point of the paraboloidal mirror M_1 lies in the equatorial plane of

the grating and half way between the slits. The distance L is very small so that both slits are very nearly at the focus of the paraboloid. Now if we consider S_1 and S_2 to be confined to the equatorial plane of the grating, so that they are essentially "point slits", then any light passing through S_1 will be rendered almost parallel by the paraboloid M_1 . These parallel rays will then make an angle δ with the vertical plane through the axis of the paraboloid, where

$$\delta = \frac{L}{f}, \quad (\text{II}, 2)$$

f being the focal length of the paraboloid.

If a point source were placed at the focal point of the paraboloid, then the parallel beam returning from M_1 would be reflected by M_2 striking the grating at some angle $\alpha = \theta$, and the light returning at the angle $\beta = -\theta$ would be again focused at the focal point of the paraboloid. Now light from S_1 will be incident on the grating at an angle

$$\alpha = \theta - \delta, \quad (\text{II}, 3)$$

and the light returning at an angle

$$\beta = -(\theta + \delta) \quad (\text{II}, 4)$$

will be focused at S_2 .

If these values of α and β are substituted into the grating equation then

$$m\lambda = d[\sin(\theta - \delta) + \sin(\theta + \delta)], \quad (\text{II}, 5)$$

which may be reduced to

$$m\lambda = 2d \cos \delta \sin \theta. \quad (\text{II}, 6)$$

For infrared work this equation is more useful in terms of wave numbers, $\tilde{\nu}$. The relation between λ and $\tilde{\nu}$ is

$$\tilde{\nu} = \frac{1}{\lambda} . \quad (\text{II}, 7)$$

Thus the grating equation becomes

$$\tilde{\nu} = \frac{mK_g}{\sin \theta} , \quad (\text{II}, 8)$$

where

$$K_g = \frac{1}{2d \cos \delta} . \quad (\text{II}, 9)$$

For the present system $f = 48$ inches and $L = .567$ inches, so that $\delta = \frac{L}{f} = .0118$ radians, and $\cos \delta = .99993$.

If N' is the number of lines per centimeter ruled on the grating face, then $N' = \frac{1}{d}$ and $K_g = .50004N'$.

Theoretical Resolving Power of a Grating

The resolving power, R , of a grating is defined by the relation $R = \frac{\lambda}{\delta\lambda}$ where $\delta\lambda$ is the smallest wavelength difference that the grating will resolve, and λ is the mean wavelength of the lines being resolved. If the diffraction grating has a total of N equally spaced rulings, then the condition for the principal interference maxima² of wavelength λ is that the path difference Δ of the two rays diffracted from the extreme ends of the grating equals $m\lambda$, and the condition for the first interference minimum³ is $\Delta = \frac{(mN \pm 1)\lambda}{N}$. If we assume the Rayleigh criterion, then two lines of wavelength λ and $\lambda + \delta\lambda$ are just resolved if the principal interference maximum of

²Ibid., p. 323.

³Ibid., p. 324.

one falls at the first interference minimum of the other; thus the two lines are just resolved if

$$\frac{(mN \pm 1)\lambda}{N} = m(\lambda + \delta\lambda), \quad (\text{II},10)$$

or

$$\pm \lambda = mN\delta\lambda. \quad (\text{II},11)$$

Thus

$$R = \frac{\lambda}{\delta\lambda} = \pm mN. \quad (\text{II},12)$$

In infrared work it is often more convenient to express resolving power in terms of the wave number difference, $\Delta\tilde{\nu}$, between two lines that are just resolved. $\Delta\tilde{\nu}$ is referred to as the resolution number, or simply resolution, of the grating and can be calculated as follows:

$$\frac{\tilde{\nu}}{\Delta\tilde{\nu}} = - \frac{\lambda}{\delta\lambda} = mN; \quad (\text{II},13)$$

$$\Delta\tilde{\nu} = \frac{\tilde{\nu}}{mN} = \frac{K\tilde{\nu}}{N \sin \theta}; \quad (\text{II},14)$$

$$\Delta\tilde{\nu} = \frac{1}{2Nd \cos \delta \sin \theta}. \quad (\text{II},15)$$

But $\cos \delta \approx 1$, and Nd is equal to the width of the ruled area of the grating, W , therefore,

$$\Delta\tilde{\nu} \approx \frac{1}{2W \sin \theta}. \quad (\text{II},16)$$

For the present system the gratings have $W \approx 20$ cm. Figure 4 is a graph of the theoretical resolution number for $W = 20$ cm. and for values of θ from 20° to 60° .

In practice it is not possible to produce perfect gratings because there are always slight irregularities in the grooves themselves, in the groove spacings, and in the quality of the optical flat upon which they are ruled. However, in spite of the many dif-

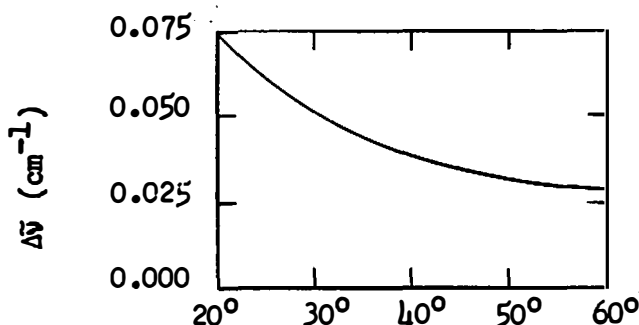


Figure 4. Resolution number

difficulties encountered in the production of reflection gratings, it is at present possible to obtain gratings which have resolving powers of the order of 80 to 90 per cent of their theoretical resolving power. The size of these gratings is, however, limited by the physical properties of the ruling engines, so that it is not always possible to obtain as large a grating (resolving power) as one would like.

Theory of Small Rotations of a Grating⁴

In order to design an adequate grating monochromator it is necessary to know what effects result from rotating the grating through a small angle about one of its axes.

Rotation About the Y-axis

It is evident that rotation about the Y-axis raises or lowers the spectrum with respect to the incident beam of light, Figure 1.

⁴R. A. Sawyer, Experimental Spectroscopy (Prentice Hall, Inc., New York, 1951), Chap. 7.

The amount of the shift can be easily calculated by considering the relative position of a "point slit" and the resulting "point images" with respect to the XY or equatorial plane. We shall consider only small rotations through an angle σ so that the "point slit" and "point image" may still be considered to lie at the focal point of the paraboloidal mirror, Figure 3.

If the grating monochromator is in perfect adjustment the equatorial plane of the grating coincides with the central plane of the spectrograph. The central plane is defined as that plane which contains the center of the paraboloidal mirror, the focal point of the paraboloidal mirror, the center of the entrance and exit slits, and the center of the grating. If the grating is turned about the Y-axis by a small angle σ , then the equatorial plane of the grating also makes an angle σ with the central plane of the spectrograph and the Y-axis of the grating is the line of intersection of the two planes, Figure 5.

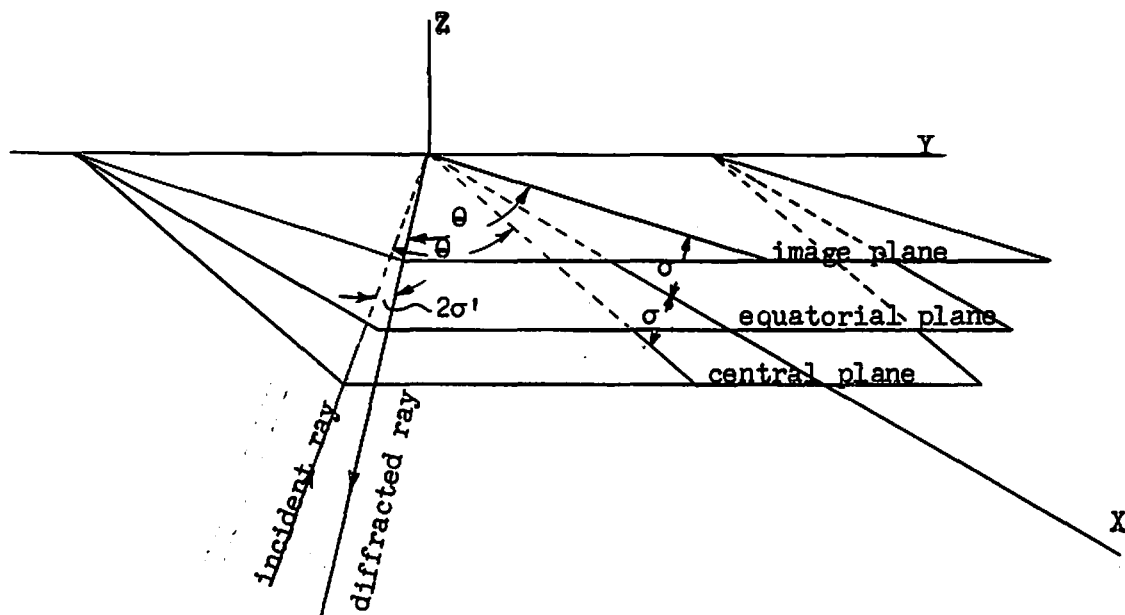


Figure 5. Rotation about the Y-axis

Collimated light from the "point" entrance slit is now incident on the grating and parallel to the central plane of the spectrograph, but it makes an angle σ' with the equatorial plane. If a ray from this collimated beam is incident on the grating at an angle θ to the normal plane, then the diffracted ray leaving the grating at the angle θ will be imaged above the exit slit of the spectrograph (for coincident entrance and exit slits). It is evident that the diffracted ray upon leaving the grating is parallel to a plane which passes through the Y-axis and makes an angle 2σ with the central plane of the spectrograph. The angle between the incident and diffracted rays, however, is not 2σ , but is an angle $2\sigma'$ which is less than 2σ except at central image. The relationship between σ' and σ is

$$\tan \sigma' = \tan \sigma \cos \theta, \quad (\text{II},17)$$

or

$$\sigma' = \tan^{-1} (\tan \sigma \cos \theta). \quad (\text{II},18)$$

The vertical displacement from the central plane of the spectral image passing through the exit slit arising from this rotation of the grating about the Y-axis is determined by the angle $2\sigma'$ which the diffracted ray makes with the central plane of the spectrograph. The diffracted ray returns making an angle $2\sigma'$ with the axis of the paraboloidal mirror, and it is thus imaged very slightly out of focus on the exit slit at a point displaced from the central plane by an amount

$$z = f \tan 2\sigma'. \quad (\text{II},19)$$

Using the trigonometric identity $\tan 2x = \frac{2 \tan x}{1 - \tan^2 x}$ and substituting from equation (II,17), one obtains

$$z = \frac{2f \tan \sigma \cos \theta}{1 - \tan^2 \sigma \cos^2 \theta} \quad (\text{II},20)$$

where f = focal length of the paraboloid.

In addition to being very slightly out of focus, the definition of the spectral line is also damaged by astigmatism, coma, and curvature.⁵

It is now evident that in order to obtain maximum resolving power the equatorial plane of the grating must be made to coincide as nearly as possible with the central plane of the spectrograph. For small deviations of the equatorial plane from the central plane, a small displacement, z , of the spectral image will result (assuming the other optics to be in perfect adjustment). Now since the angle σ is small, $\tan \sigma \approx \sigma$, and $\sigma^2 \ll 1$ so that the maximum displacement of the spectral image from the central plane (which occurs at central image, $\theta = 0$), as given by equation (II,20), will become

$$z \approx 2f\sigma. \quad (\text{II}, 21)$$

Now if it is required that z be less than 0.1 inches, this sets tolerance limits on the grating spindle depending on the focal length, f , of the collimating mirror.

For the present system $f = 48$ inches and thus the maximum deviation of the spindle axis must be less than 1.04×10^{-3} radians if the displacement of the spectral image is not to exceed 0.1 inches.

Rotation About the X-axis

If the spectrograph is in perfect alignment, then both the "point" entrance slit and the spectral images lie in the central plane of the spectrograph; however, if the grating is rotated about

⁵Ibid., p. 87.

the X-axis by an angle ω , then the equatorial plane of the grating also makes an angle ω with the central plane of the spectrograph, and the intersection of the two planes is the X-axis, Figure 6. The diffracted rays now return from the grating parallel to the plane determined by the directly reflected beam and the Y-axis. The true angle of incidence, θ , which is the angle between the incident ray and the normal plane, is no longer equal to the angle of incidence as measured in the central plane, θ' ; but if ω is small, θ is very nearly equal to the angle determined by projecting the incident ray onto the equatorial plane. It will be assumed here for simplicity that these angles are equal.

The relationship between θ and θ' may then be derived from Figure 6 as follows:

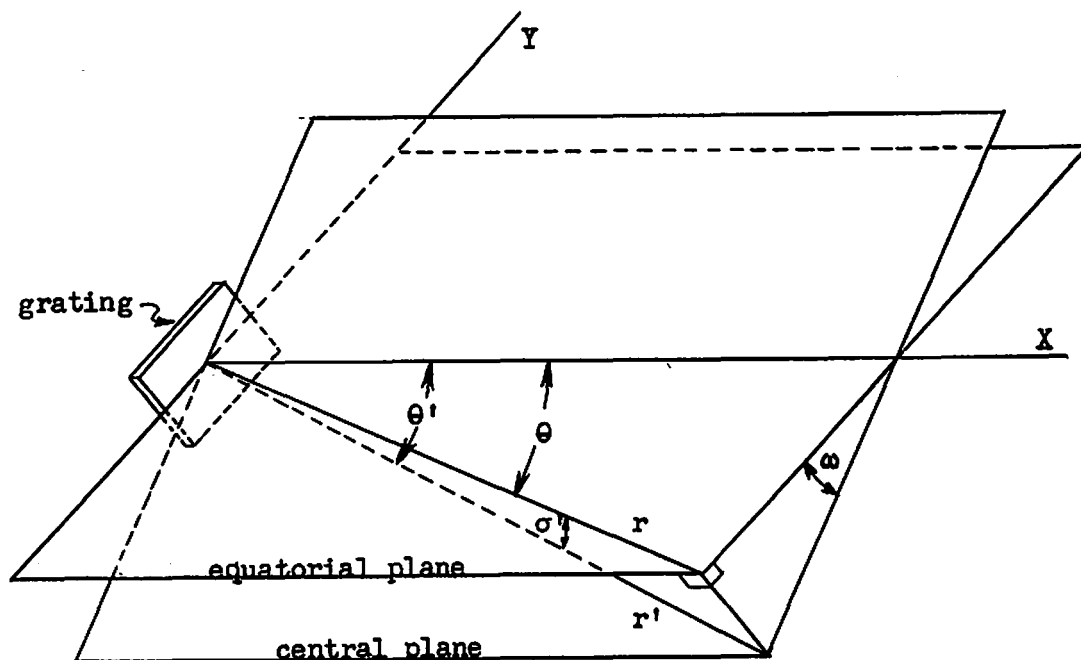


Figure 6. Rotation about the X-axis

$$r \sin \theta = r' \sin \theta' \cos \omega \quad (\text{II}, 22)$$

$$r \cos \theta = r' \cos \theta' \quad (\text{II}, 23)$$

Dividing the first equation by the second one obtains the relationship

$$\tan \theta = \tan \theta' \cos \omega \quad (\text{II}, 24)$$

or

$$\theta = \tan^{-1} (\tan \theta' \cos \omega). \quad (\text{II}, 25)$$

Thus $\theta \leq \theta'$ for $0 < \theta < \pi/2$ and if the spectrograph is set at the angle θ' the wavelength falling on the exit slit will be shorter than the wavelength calculated by using θ' in the grating equation.

It can be seen from Figure 6 that the "point slit" is now at an angle σ' below the equatorial plane, and the spectral image is at an angle σ' above it.

The value of σ' may be derived as follows:

$$r = r' \cos \sigma' \quad (\text{II}, 26)$$

$$r \sin \theta = r' \sin \theta' \cos \omega. \quad (\text{II}, 27)$$

Dividing the first equation by the second one obtains

$$\frac{1}{\sin \theta} = \frac{\cos \sigma'}{\sin \theta' \cos \omega} \quad (\text{II}, 28)$$

or

$$\cos \sigma' = \frac{\sin \theta' \cos \omega}{\sin \theta}. \quad (\text{II}, 29)$$

Substituting from equation (II, 25) for θ one obtains

$$\cos \sigma' = \frac{\sin \theta' \cos \omega}{\sin [\tan^{-1} (\tan \theta' \cos \omega)]} \quad (\text{II}, 30)$$

$$\sigma' = \cos^{-1} \left\{ \frac{\sin \theta' \cos \omega}{\sin [\tan^{-1} (\tan \theta' \cos \omega)]} \right\} \quad (\text{II}, 31)$$

The displacement of the spectral image is again given by equation (II, 19), and the image is again slightly out of focus at the exit slit.

For $0 \leq \theta \leq \pi/2$ and $-\pi/2 \leq \omega \leq \pi/2$,

$$\tan \theta' \geq \tan \theta' \cos \omega \quad (\text{II},32)$$

and

$$\sigma' \leq \cos^{-1} \left\{ \frac{\sin \theta' \cos \omega}{\sin [\tan^{-1} (\tan \theta')]} \right\}, \quad (\text{II},33)$$

which reduces to

$$\sigma' \leq \omega. \quad (\text{II},34)$$

Thus, as far as spindle design is concerned, this type of rotation imposes tolerances of the same size as those imposed by rotation about the Y-axis.

In actual practice slits of finite length are used. These slits are adjusted so as to be perpendicular to the central plane of the spectrograph. If the slits are short compared to the focal length of the collimator, then it can be assumed, without making a serious error, that light entering from any point of the entrance slit is incident on the grating at the same angle as light entering from the center of the slit. However, if the slits are inclined at an angle ω to the rulings of the grating, it is evident that each point of the entrance slit lies at a different angle of incidence, and, therefore, for each point the angle of diffraction for constant λ will be different. If the slit is of length b and the angle ω is small, and if the center of the entrance slits is taken to lie in the equatorial plane at an angle α_0 to the grating, then one end of the slit makes an angle $\alpha^+ = \alpha_0 + \Delta\alpha$ with the grating, and the other end makes an angle $\alpha^- = \alpha_0 - \Delta\alpha$ with it. The angle $\Delta\alpha$ is now a function of the focal length of the paraboloid given by

$$\Delta\alpha = \frac{b\omega}{2f}. \quad (\text{II}, 35)$$

If it is assumed that $\Delta\alpha$ is positive for the top of the entrance slit and negative for the bottom, then

$$\alpha^+ = \alpha_0 + \frac{b\omega}{2f} \quad (\text{II}, 36)$$

and

$$\alpha^- = \alpha_0 - \frac{b\omega}{2f}. \quad (\text{II}, 37)$$

Now light entering through the top of the entrance slit at an angle α^+ will be diffracted by the grating and imaged at the bottom of the exit slit at an angle β^- .

If the grating equation (II,1) is written

$$\sin \beta = \sin \alpha - \frac{m\lambda}{d}, \quad (\text{II}, 38)$$

then for the top of the entrance slit equation (II,38) becomes

$$\sin \beta^- = \sin \left(\alpha_0 + \frac{b\omega}{2f} \right) - \frac{m\lambda}{d}, \quad (\text{II}, 39)$$

and for the bottom of the entrance slit equation (II,38) becomes

$$\sin \beta^+ = \sin \left(\alpha_0 - \frac{b\omega}{2f} \right) - \frac{m\lambda}{d}. \quad (\text{II}, 40)$$

If the substitutions

$$\beta^+ = \beta_0 + \Delta\beta \quad (\text{II}, 41)$$

and

$$\beta^- = \beta_0 - \Delta\beta \quad (\text{II}, 42)$$

are now made and equation (II,40) is subtracted from equation (II,39), one obtains

$$\begin{aligned} & \sin (\beta_0 - \Delta\beta) - \sin (\beta_0 + \Delta\beta) \\ &= \sin \left(\alpha_0 + \frac{b\omega}{2f} \right) - \sin \left(\alpha_0 - \frac{b\omega}{2f} \right), \quad (\text{II}, 43) \end{aligned}$$

which may be reduced to

$$-\cos \beta_0 \sin \Delta\beta = \cos \alpha_0 \sin \frac{b\omega}{2f}. \quad (\text{II}, 44)$$

If it is assumed that the entrance and exit slits coincide, then

$$\alpha_0 = -\beta_0 = \theta_0, \quad (\text{II}, 45)$$

and, therefore,

$$-\sin \Delta\beta = \sin \frac{b\omega}{2f}, \quad (\text{II}, 46)$$

and

$$\Delta\beta = -\frac{b\omega}{2f}, \quad (\text{II}, 47)$$

so that equations (II, 41) and (II, 42) become

$$\beta^+ = \beta_0 - \frac{b\omega}{2f} \quad (\text{II}, 48)$$

and

$$\beta^- = \beta_0 + \frac{b\omega}{2f}. \quad (\text{II}, 49)$$

Comparing equation (II, 48) with equation (II, 36) and substituting equation (II, 45) it is seen that

$$\alpha^+ = \theta_0 + \frac{b\omega}{2f} = -\beta^+, \quad (\text{II}, 50)$$

and similarly

$$\alpha^- = \theta_0 - \frac{b\omega}{2f} = -\beta^-. \quad (\text{II}, 51)$$

This means that the diffracted image of wavelength λ is slanted with respect to the rulings of the grating in the same direction as the entrance slit, and, therefore, the entire image passes through the exit slit. Thus this type of misalignment has only a small effect on the resolving power of the instrument, and the tolerance to which the spindle must be held is determined by the effect of rotating the grating about the X and Y axes. Therefore, the maximum deviation of

the spindle axis must be less than 10^{-3} radians, as was shown on page 15.

Theory of Slit Curvature

Thus far it has been assumed that a straight entrance slit will produce a straight spectral image. This, however, is not the case. When a straight slit of finite length is used, the spectral lines are slightly curved⁶ because a ray coming through the entrance slit at a point above the central plane does not approach the grating in the equatorial plane but from an angle σ'_a above this plane, Figure 7, and the diffracted ray will return at an angle $-\sigma'_\beta$. (It is assumed here that the central plane and equatorial plane coincide.) To these rays the angles of incidence, α' , and diffraction, β' , are less than the angles of incidence, α , and diffraction, β , in the equatorial

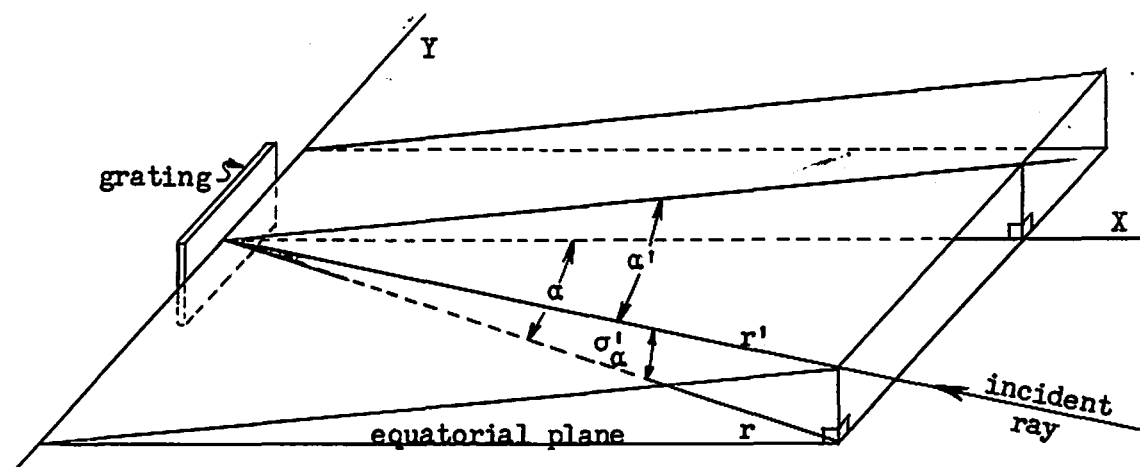


Figure 7. Ray incident from finite entrance slit

⁶H. M. Randall and F. A. Firestone, Rev. Sci. Inst. 9, 407 (1938).

plane. The grating equation is now written

$$m\lambda = d(\sin \alpha' - \sin \beta'), \quad (\text{II}, 52)$$

where α' and β' are now functions of the slit position through which the light passes.

It can be seen from Figure 7 that

$$r = r' \cos \sigma_{\alpha}', \quad (\text{II}, 53)$$

and

$$r \sin \alpha = r' \sin \alpha'. \quad (\text{II}, 54)$$

Substituting (II,53) into (II,54) one obtains

$$\sin \alpha' = \sin \alpha \cos \sigma_{\alpha}'. \quad (\text{II}, 55)$$

Similarly

$$\sin \beta' = \sin \beta \cos \sigma_{\beta}'. \quad (\text{II}, 56)$$

If a ray passes through the entrance slit at a distance z_{α} from the equatorial plane and the distance z_{α} is small compared to the focal length, f , of the collimator, then the angle σ_{α}' is given by

$$\sigma_{\alpha}' = \frac{z_{\alpha}}{f}, \quad (\text{II}, 57)$$

and

$$\sigma_{\beta}' = \frac{z_{\beta}}{f}, \quad (\text{II}, 58)$$

where z_{α} and z_{β} vary from $-\frac{b}{2}$ to $\frac{b}{2}$.

The grating equation for a spectrograph having slits of finite length may then be written

$$m\lambda = d\left(\sin \alpha \cos \frac{z_{\alpha}}{f} - \sin \beta \cos \frac{z_{\beta}}{f}\right). \quad (\text{II}, 59)$$

In the present instrument the sensitive element of the detector is straight, and it is, therefore, desirable to have a straight exit

slit so that the entire image will fall on the detector. Thus one wishes to curve the entrance slit so as to produce a straight spectral image. This means that we wish to obtain an image of constant λ at the angle β . Thus α will be a function of z_α and z_β , but β will be independent of z_α and z_β .

If α is very nearly equal to $-\beta$, then it is evident that a ray passing through the entrance slit at a distance z_α above the equatorial plane will be imaged on the exit slit at a distance $-z_\beta$ below the equatorial plane. Thus

$$z_\alpha = -z_\beta = z, \quad (\text{II}, 60)$$

and equation (II,59) becomes

$$m\lambda = d \left[\cos \frac{z}{f} \right] (\sin \alpha - \sin \beta). \quad (\text{II}, 61)$$

To obtain an image of constant λ at the angle β , $\frac{d\lambda}{dz}$ must vanish. Differentiating equation (II,61) with respect to z , one obtains

$$\begin{aligned} m \frac{d\lambda}{dz} = d \left[-\frac{1}{f} \sin \frac{z}{f} (\sin \alpha - \sin \beta) \right. \\ \left. + \cos \frac{z}{f} \cos \alpha \frac{d\alpha}{dz} \right] = 0, \end{aligned} \quad (\text{II}, 62)$$

or

$$\frac{d\alpha}{dz} = \frac{1}{f} \tan \frac{z}{f} \frac{(\sin \alpha - \sin \beta)}{\cos \alpha}. \quad (\text{II}, 63)$$

As discussed earlier, the entrance and exit slits in the present system are separated at the equatorial plane by a small distance $2L$, Figure 3; and the angles of incidence and diffraction in the equatorial plane are related by equation (II,3) and (II,4). For a curved entrance slit and points above or below the equatorial plane, these

equations may be written

$$\alpha = \theta - \delta_{\alpha} \quad (\text{II}, 64)$$

and

$$\beta = -(\theta + \delta_{\beta}), \quad (\text{II}, 65)$$

where δ_{α} is defined by

$$\delta_{\alpha} = \frac{L_{\alpha}}{f} \quad (\text{II}, 66)$$

and δ_{β} is defined by

$$\delta_{\beta} = \frac{L_{\beta}}{f} \quad (\text{II}, 67)$$

and where θ is the grating setting relative to central image. L_{α} is the horizontal distance from a vertical plane passing through the axis of the collimating mirror to a point in the entrance slit at a distance z from the equatorial plane, Figure 8. Since the entrance slit is curved, δ_{α} and L_{α} are both functions of z . L_{β} is the horizontal

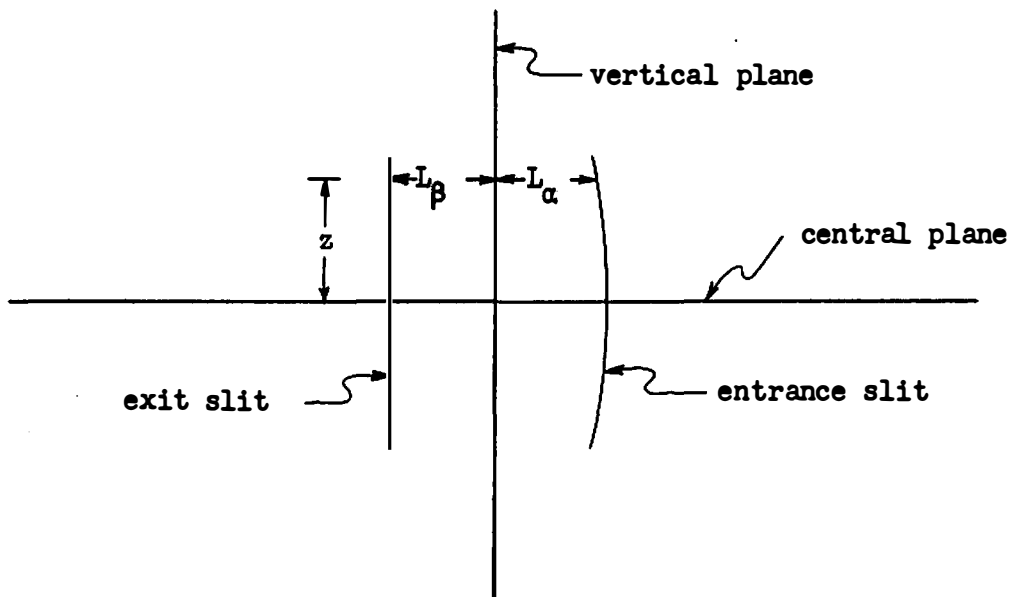


Figure 8. Slit system

distance from the same vertical plane to a point in the exit slit at a distance z from the equatorial plane, but L_β is a constant because the exit slit is straight. Now δ_α and δ_β are both small so that

$$\sin \delta_\alpha \approx \tan \delta_\alpha \approx \delta_\alpha = \frac{L_\alpha}{f}, \quad (\text{II}, 68)$$

$$\sin \delta_\beta \approx \tan \delta_\beta \approx \delta_\beta = \frac{L_\beta}{f}, \quad (\text{II}, 69)$$

and

$$\cos \delta_\alpha \approx \cos \delta_\beta \approx 1. \quad (\text{II}, 70)$$

also z is small compared to f , so that

$$\tan \frac{z}{f} \approx \frac{z}{f}. \quad (\text{II}, 71)$$

Substituting equations (II, 64) and (II, 65) into equation (II, 63) one obtains

$$-\frac{d\delta_\alpha}{dz} = \frac{1}{f} \tan \frac{z}{f} \left[\frac{\sin (\theta - \delta_\alpha) + \sin (\theta + \delta_\beta)}{\cos (\theta - \delta_\alpha)} \right]. \quad (\text{II}, 72)$$

Using the trigonometric relations for the sum of two angles together with equations (II, 68) through (II, 71), one may obtain the equation

$$\frac{dL_\alpha}{dz} = -\frac{z}{f} \left[\frac{2 \tan \theta + \frac{L_\beta - L_\alpha}{f}}{1 + \frac{L_\alpha}{f} \tan \theta} \right]. \quad (\text{II}, 73)$$

Now L_α is approximately equal to L_β , and thus $\frac{L_\beta - L_\alpha}{f}$ is very small and becomes negligible compared to $\tan \theta$ over the useful range of the grating ($20^\circ < \theta < 60^\circ$). Thus equation (II, 73) may be rewritten in integrable form as

$$-\int_L^{L_\alpha} \left(1 + \frac{L_\alpha}{f} \tan \theta \right) dL_\alpha = \frac{2}{f} \tan \theta \int_0^z z \, dz. \quad (\text{II}, 74)$$

The term $\frac{L_a}{f} \tan \theta$ on the left hand side of equation (II, 74) is the term resulting from the fact that the entrance and exit slits are separated by a small distance. If this term is neglected, then the equation holds for entrance and exit slits which coincide at the equatorial plane, and integration yields

$$L - L_a = \frac{z^2}{f} \tan \theta, \quad (\text{II, 75})$$

which is the result obtained by Randall and Firestone⁷.

Integrating equation (II, 74) one may obtain

$$(L - L_a) \left(1 + \frac{L + L_a}{2f} \tan \theta\right) = \frac{z^2}{f} \tan \theta. \quad (\text{II, 76})$$

Now L is approximately equal to L_a , so that

$$L + L_a \approx 2L, \quad (\text{II, 77})$$

and thus equation (II, 76) becomes

$$L - L_a = \frac{\frac{z^2}{f} \tan \theta}{\left(1 + \frac{L}{f} \tan \theta\right)}. \quad (\text{II, 78})$$

From equation (II, 78) it can be seen that the entrance slit should be straight at central image ($\theta = 0$) and become increasingly curved as θ increases. Thus it would be desirable to have an entrance slit of variable curvature. This, however, is not too practical, and one usually curves the entrance slit for an angle in the center of the useful region of the grating, i.e. about forty degrees.

It is also convenient to approximate the slit curvature by the arc of a circle, Figure 9.

From the Pythagorean theorem it can be seen that

⁷Loc. cit.

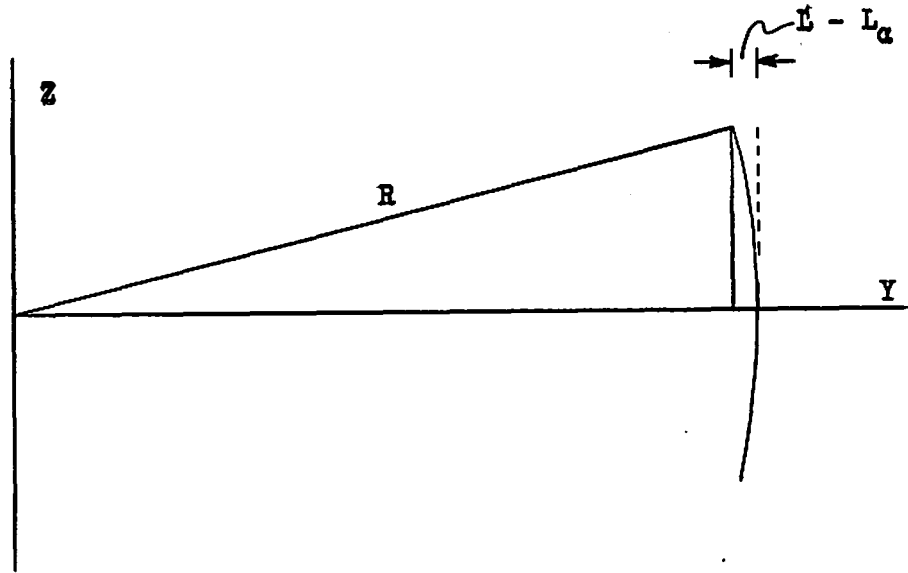


Figure 9. Slit curvature as an arc of a circle

$$R^2 = z^2 + (R - L + L_\alpha)^2, \quad (\text{II}, 79)$$

where R is the radius of curvature of the arc. This may be reduced to

$$R = \frac{z^2}{2(L - L_\alpha)} + \frac{L - L_\alpha}{2}. \quad (\text{II}, 80)$$

Upon substitution of equation (II, 78), equation (II, 80) becomes

$$R = \frac{f}{2} \left(\cot \theta + \frac{L}{f} \right) + \frac{z^2 \tan \theta}{2f \left(1 + \frac{L}{f} \tan \theta \right)}. \quad (\text{II}, 81)$$

For the useful range of the spectrograph and for short slits, the second term of equation (II, 81) is small compared to the first and may be neglected. Thus it is possible to approximate the slit curvature by an arc of a circle of radius

$$R = \frac{f}{2} \left(\cot \theta + \frac{L}{f} \right). \quad (\text{II}, 82)$$

In the present system the focal length of the collimator, f , is forty-eight inches, the slit separation in the equatorial plane $2L$ is 1.13 inches, and the slit is curved for forty degrees so that $R = 28.91$ inches.

Characteristics of the Fabry-Perot Interferometer

The Fabry-Perot Interferometer^{8,9} is a device which produces interference fringes by multiple reflection of light in a thin gap between two partially silvered parallel plates. The condition for constructive interference is

$$m\lambda = 2d \cos \theta. \quad (\text{II}, 83)$$

where d is the thickness of the gap, θ is the angle that an incident ray makes with the axis of the parallel plates, λ is the wavelength of the incident light, and m is an integer, (see Figure 10). If equation (II,83) is rewritten in terms of wave numbers, $\tilde{\nu}$, it becomes

$$\tilde{\nu} = \frac{1}{\lambda} = \frac{m}{2d \cos \theta} \quad (\text{II}, 84)$$

When a pair of Fabry-Perot plates are mounted with a constant spacing, d , the system is referred to as an etalon. The wave number spacing of the etalon's interference maxima, $\Delta\tilde{\nu}$, is determined by the plate spacing, d .

If d and θ are held constant and the wave number of the incident light is changed from one state of constructive interference, $\tilde{\nu}_m$, to

⁸F. A. Jenkins and H. E. White, op. cit., Chap. 14.

⁹S. Tolansky, High Resolution Spectroscopy (Pitman Publishing Corporation, New York, 1947), Chap. 7.

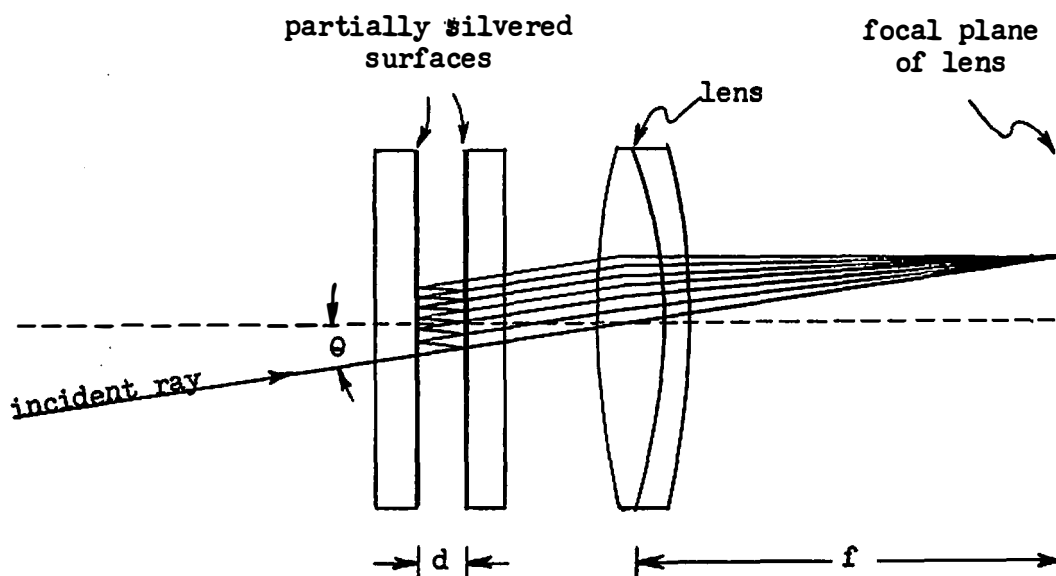


Figure 10. The Fabry-Perot Interferometer

the next, $\tilde{\nu}_m + 1$, then the change in wave number, $\Delta\tilde{\nu}$, is given by

$$\Delta\tilde{\nu} = \tilde{\nu}_m + 1 - \tilde{\nu}_m = \frac{1}{2d \cos \theta}, \quad (\text{II}, 85)$$

and the wave number spacing, $\Delta\tilde{\nu}$, between successive interference maxima remains constant as $\tilde{\nu}$ is varied.

This constant wave number spacing can then be used as a "yard-stick" for measuring the wave number difference between spectral lines by recording the etalon pattern and infrared spectrum simultaneously on the same chart. Absolute wave number measurements may then be obtained by putting a well known emission or absorption line on the chart to provide a standard line from which to measure.

CHAPTER III

DETAILS OF DESIGN AND CONSTRUCTION

The Vacuum System

The prism and grating monochromators, Fabry-Perot etalon, sources, detectors, and associated hardware, which constitute the spectrometer proper, are mounted on the spectrometer table which is cantilevered from the front end of a large steel vacuum tank, Figures 11 and 12; while the spectrometer controls, amplifiers, and power supplies are mounted in relay racks outside the vacuum tank, Figure 13. The double pen recorder is shown, Figure 12, beside the open vacuum tank.

The Vacuum Tank

The vacuum housing is a cylindrical steel tank built for this job by Combustion Engineering, Inc. of Chattanooga, Tennessee. It is about five feet in diameter and seven and a half feet long having a volume of about 134 cubic feet or 1000 gallons. The tank is built in two sections which are sealed vacuum tight by means of a neoprene gasket. Figure 11 is a view of the tank showing the front and one side. The tank separates near the front end, and the rear section is mounted on wheels and may be rolled back exposing the spectrometer table, Figure 12. The front end is supported by two vertical half inch steel plates welded to it and to the base plate. The two sections of the tank are provided with lugs so that the tank may be bolted

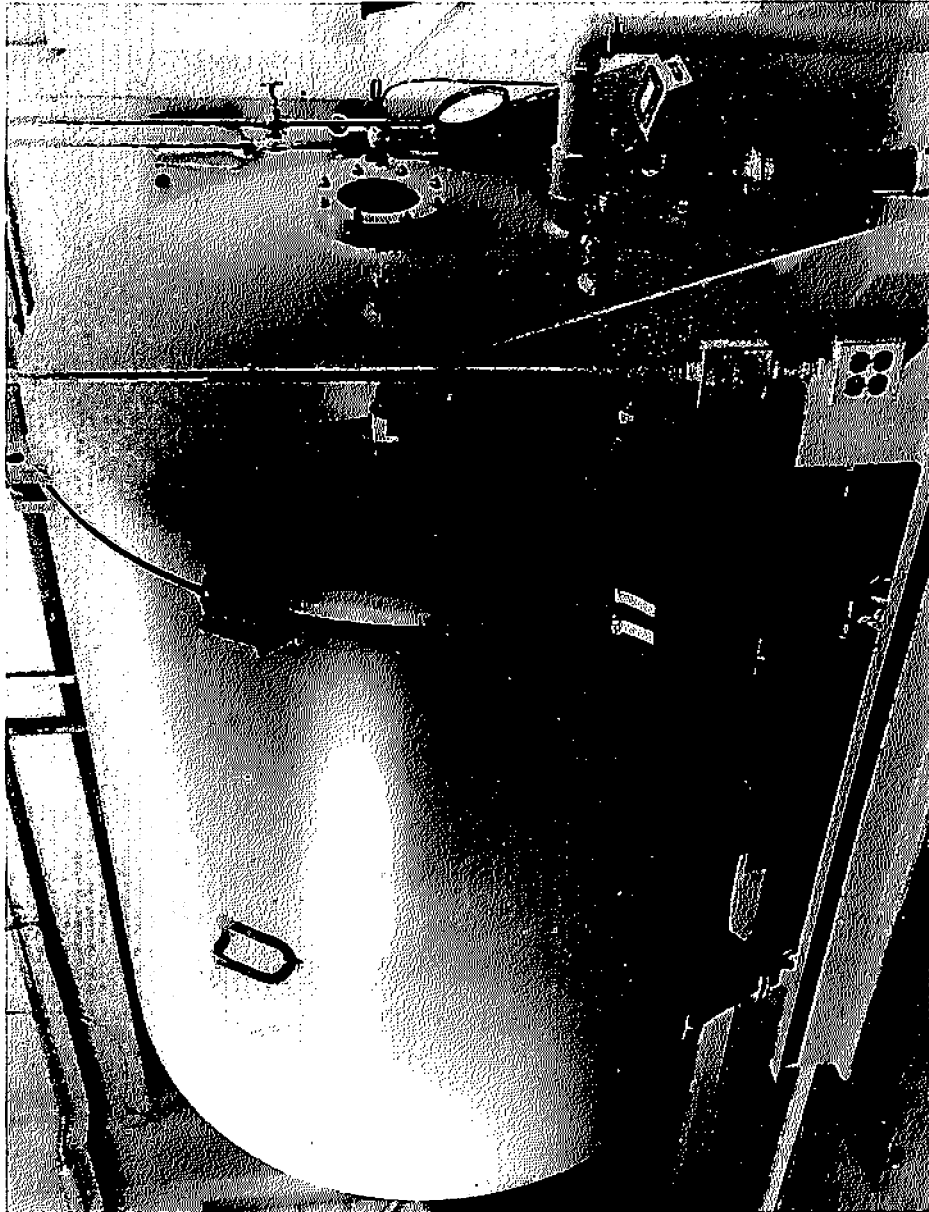


Figure 11. Vacuum tank with rear section in place

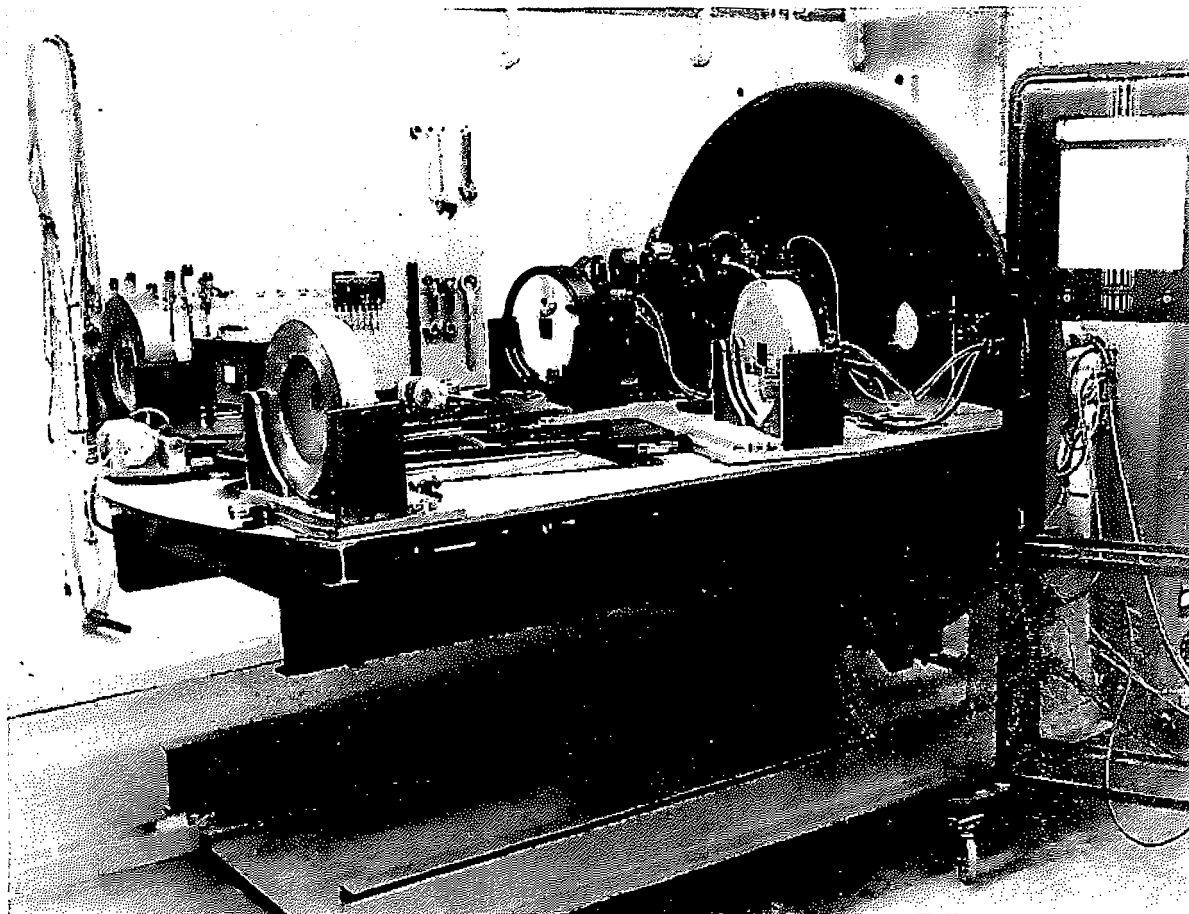


Figure 12. Vacuum tank with rear section removed exposing the spectrometer table

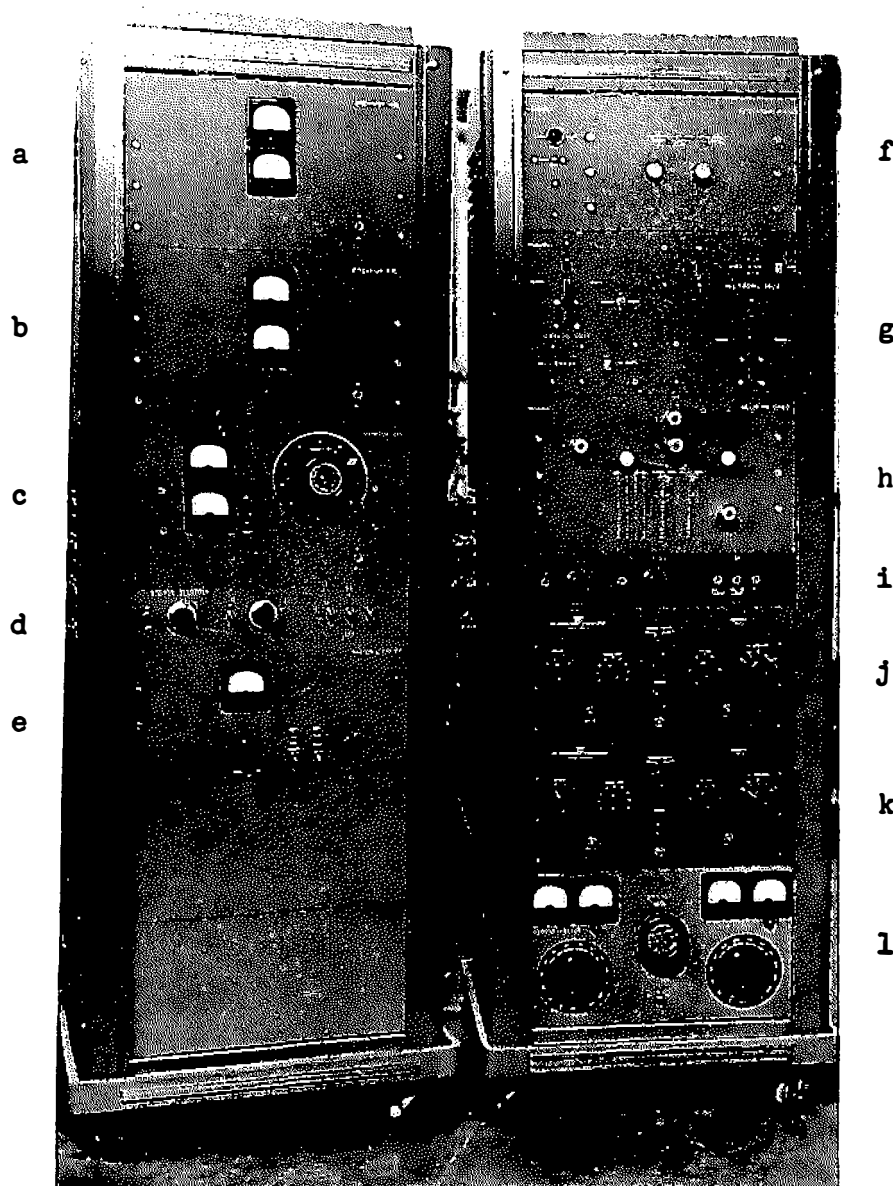


Figure 13. Spectrometer controls, a) and b) zirconium arc power supplies, c) krypton arc power supply, d) control panel with source selector, e) photomultiplier power supply, f) positioning drive, g) positioning drive and scanning drive control panel, h) scanning drive, i) slit width and prism monochromator control panel, j) and k) Model 107 amplifiers, l) Nernst glower and heater power supply

closed to seal the gasket and allow the vacuum to take hold. Once a few centimeters of vacuum are obtained, the bolts may be removed.

The front end of the tank is provided with a six inch diameter pyrex window. This window may be used to observe the interior of the tank when it is under vacuum, or it may be replaced by a suitably transparent material, thus permitting the use of external infrared sources. There are also twelve ports in the tank made by welding one inch pipe couplings into the front end. Most of these ports are fitted with hermetically sealed electrical connectors which make it possible to get the electrical control cables into the vacuum. One of the ports is fitted with vacuum gauges and coolant lines, and others may be used for controlling the pressure of samples being studied.

The front end of the tank is also fitted with a two inch vacuum pump line through which the air is pumped from the system. Air is admitted to the tank through the filter and one inch vacuum valve which project downward from the two inch pipe at the head of the tank, Figure 11. The filter serves both to remove dust from the air admitted to the tank and to reduce the flow rate to prevent "wind" damage to the spectrograph.

The Vacuum Pump

The air is removed from the tank by a Model VSD-8-8-11 Kinney vacuum pump¹ (Figure 14) having a displacement of 46.80 cubic feet per minute at 360 rpm. This pump will reduce the pressure in the

¹"Bulletin V51", (Kinney Manufacturing Co., Boston, Mass., 1953)

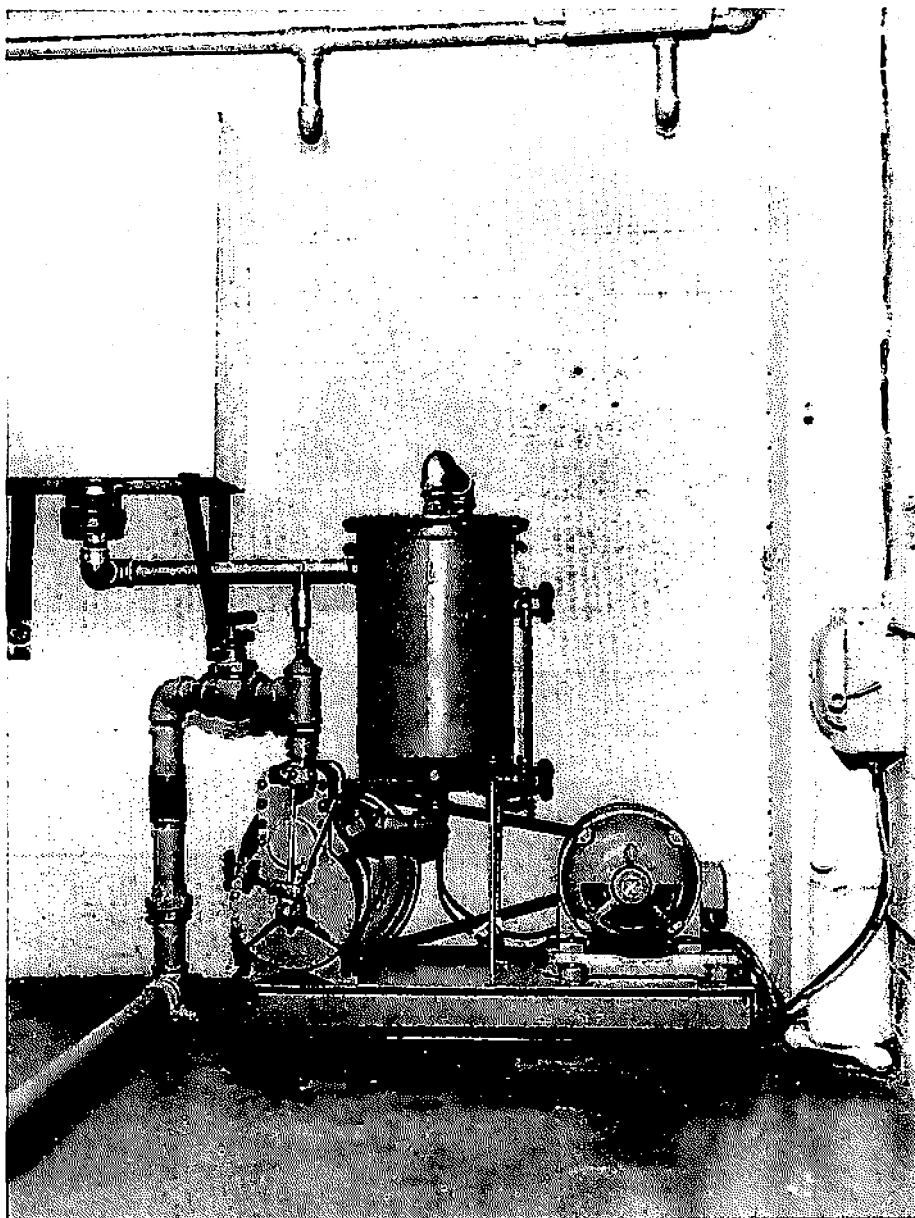


Figure 14. The vacuum pump

tank to one millimeter of mercury in about twenty-five minutes and will ultimately reduce the pressure below sixty microns if a sufficiently dry pump oil such as Kinney Super X Vacuum dried oil is used.

The tank may be shut off from the pump by means of a two inch vacuum valve located near the throat of the pump, Figure 14. When the instrument is being run, this two inch valve is normally closed and the pump is shut off to eliminate the vibration present when the pump is in operation. A Sylphon bellows in the pump line reduces the amount of vibration transmitted to the vacuum tank from the pump.

When the pump is running, air is exhausted into the laboratory through a filter which removes most of the oil mist created by the pump. A slight amount of oil mist does, however, come through. (See Appendix A for details on evacuating the spectrograph).

Vacuum Gauges

The pressure in the vacuum tank is measured by two gauges. An Ashcroft vacuum gauge covers the range up to seventy-six centimeters of mercury or about 10,000 microns total pressure, and a Hastings thermocouple gauge covers the range from 1000 microns to one micron total pressure.

Leak Detector

A freon leak detector tube is placed near the throat of the pump, and whenever changes are made which would affect the vacuum seal of the tank they are checked with this leak detector.

The Cantilever Frame and Spectrometer Table

The cantilever frame which supports the spectrometer is constructed of seven inch steel channel welded to the front end of the vacuum tank and cross braced with two inch steel angle. This cantilever frame was designed to hold one thousand pounds supported at its center.

In order to remain within the weight limitations imposed by the cantilever frame, the spectrometer table was fabricated from aluminum. The ribs for this table consist of a grid work of three inch aluminum "I" beams which were bolted together and reinforced at the joints with four inch aluminum angle. The top of this ribbing was then planed to make it flat, and two pieces of half inch aluminum tool and jig plate were screwed to it to form a flat table top.

The tool and jig plate had previously had a grid work of threaded holes tapped into it. The holes are placed four inches apart along the length of the table with the same spacing across the width. The purpose of this grid work is to allow temporary changes or experimental modifications to be made without defacing the instrument.

The table is fifty-four inches wide and has an over-all length of ninety and one half inches. It is divided in half lengthwise with one spectrograph on each half. The principal optics and drive mechanisms of the double pass spectrograph were designed to be the mirror image of the principal optics and drive mechanisms of the single pass instrument, so that these elements would be placed symmetrically with respect to the dividing line. This was done to obtain a uniform

weight distribution on the spectrometer table.

The spectrometer table is supported on the cantilever frame by three shock mounts. There are two reasons for this type of mount. First, the shock mounts reduce the amount of vibration transmitted from the room to the spectrometer table, and second, the three point suspension prevents the spectrometer table from warping when the tank is evacuated. When the air is removed from the tank large forces are applied to the tank by the atmospheric pressure in the room, and the tank becomes slightly distorted. When this distortion occurs the cantilever frame also distorts, and if the spectrometer table were attached rigidly to it, the table would also be distorted, and the optics would be thrown out of alignment.

The Single Pass Infrared Grating Monochromator

The Optical System of the Grating Monochromator

The heart of the spectrograph is, of course, the grating monochromator, Figure 15. This is a device for dispersing light into its component frequencies or colors. The monochromator used here is a modified Pfund type in which the mirrors are used twice.

Light from the prism monochromator enters the grating monochromator through slit S_2 , passes through the hole in the plane mirror M_{11} , and is collimated by the paraboloidal mirror M_{10} . The returning parallel light is then reflected to the grating by M_{11} . The light is diffracted by the grating, and a parallel beam of frequency ν is returned to M_{11} and thence to M_{10} , which focuses it on the exit

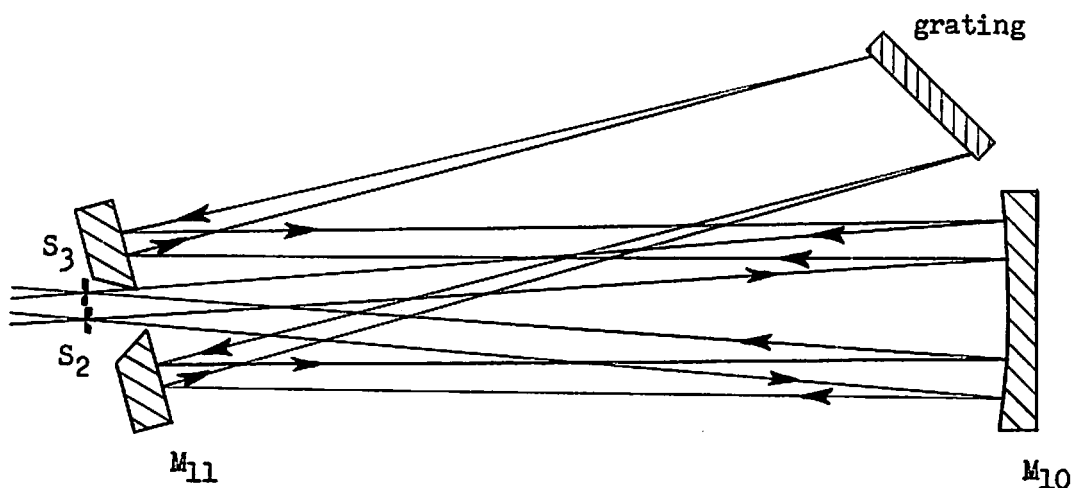


Figure 15. Diagram of the grating monochromator

slit S_3 . Upon passing through the exit slit, the light is focused on an infrared detector which controls one pen of the double pen recorder.

Mirrors and Mirror Mounts for the Grating Monochromator

All of the mirrors used in the spectrograph are front surface mirrors with a reflective coating of aluminum. This type of mirror is used because glass absorbs infrared radiation. These mirrors must be handled with extreme care to prevent the reflective coating from being marred.

The mirror blanks used in making M_{10} and M_{11} were pyrex discs twelve and a quarter inches in diameter and two inches thick. M_{10} is a high quality paraboloidal mirror with a focal length of forty-

eight inches, and M_{11} is a plane mirror which is flat to one quarter of a wavelength of sodium light. M_{11} has a hole cut in its center to allow the paraboloidal mirror M_{10} to be used on axis. This hole is tapered from a two inch square at the mirror surface to a four and a half inch square at the back.

The mirror mounts for M_{10} and M_{11} were fabricated primarily from aluminum and were designed to provide fine and accurate linear adjustment in the direction of the axis of the mirror as well as fine rotations about a vertical and a horizontal axis. All of these adjustments are made with opposing screws so that positive and reproducible motion may be obtained.

The lower plate of the mirror mount, Figure 16, rides on two ways like the carriage of a lathe. The two opposing screws fastened directly to the spectrometer table move the lower plate on the ways to provide the motion in the direction of the mirror axis. One of the opposing screws is a micrometer which makes it possible to reproduce mirror settings to one thousandth of an inch.

Set into this lower plate is a brass ring which protrudes above the surface of the plate about one quarter of an inch. The upper plate of the mirror mount which carries the yoke for the mirror holder, Figure 17, has a circular recess in the bottom which just fits the brass ring. This ring and the recess form the bearing for the motion about the vertical axis. The two plates are held together by a shoulder screw which fits through the hole in the lower plate and screws into the upper plate. The motion about the vertical axis is controlled by opposing screws in the upper plate which bear against

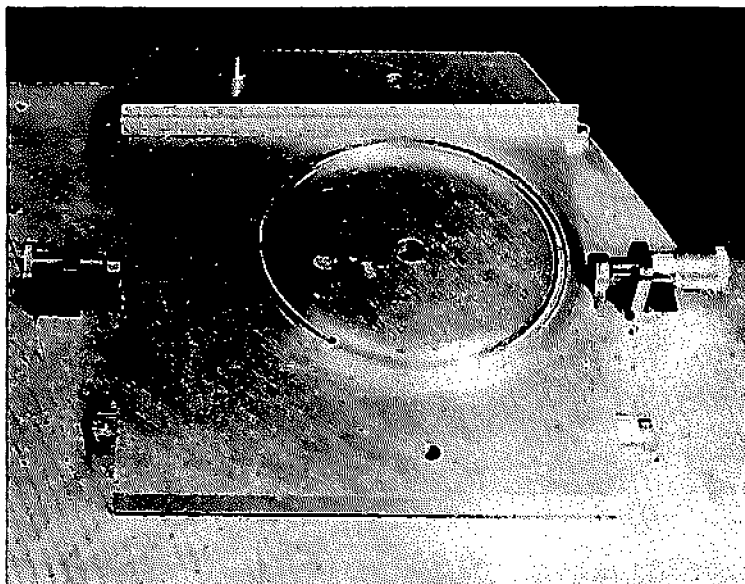


Figure 16. Lower plate of mirror mount

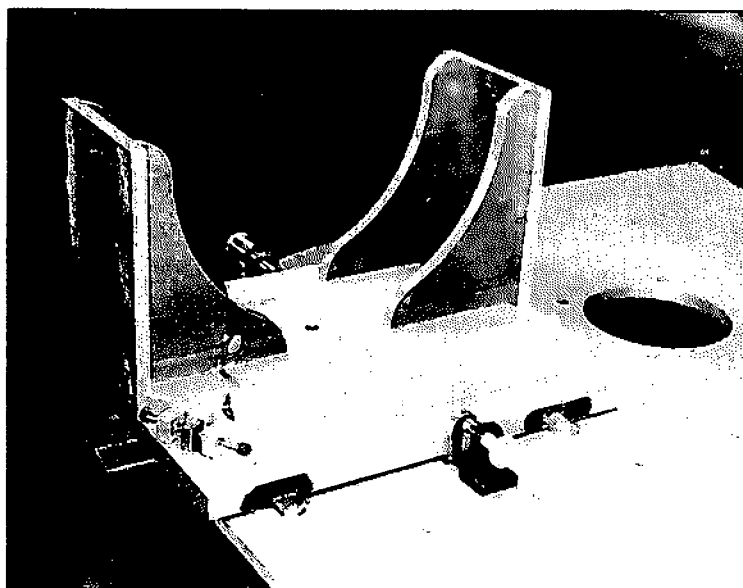


Figure 17. Mirror mount with upper plate and yoke in place

the steel post pressed into the lower plate.

Two bronze sleeve bearings are pressed into the yoke to provide the axis for rotation about the horizontal axis. Corresponding holes are drilled in the mirror holder, and the mirror holder is mounted in the yoke, Figure 18, by inserting two hardened and ground steel pins through the sleeve bearings and pressing them into the holes in the mirror holder. The hardened steel pins are drilled and tapped on the outer end so that they may be removed with a suitable puller.

The mirror holders are machined from a special aluminum casting having a hole in the back so that light may pass through the square hole in the plane mirror. The mirrors are held in place by a threaded retaining ring which screws into the front of the holder. The mirror is backed by a cork gasket to prevent chipping of the glass, and a composition fiber gasket is placed between the retaining ring and the surface of the mirror. The mirror must be assembled in the mirror holder before the mirror holder is mounted in the yoke.

The axes of horizontal and vertical rotation are chosen so that they pass through the center of mass of the mirror-mirror holder assembly. This provides vibrational stability for the mounted mirror.

The rotation about the horizontal axis is controlled by opposing screws which are located in the two braces on one side of the yoke. These screws bear against a steel block fastened to the outside of the mirror holder.

Grating Mounts

At present there are four gratings available for use with the

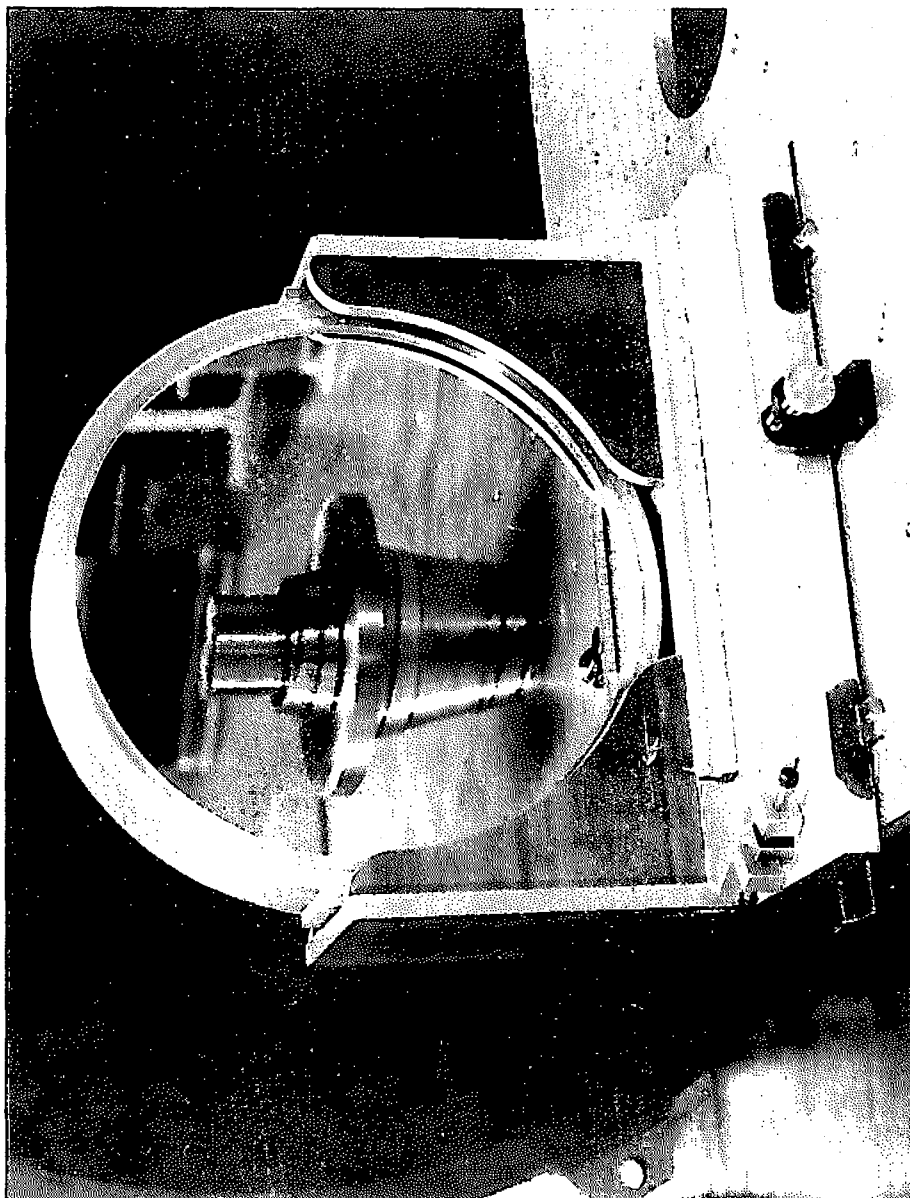


Figure 18. Mirror mount with mirror holder and mirror in place

spectrograph (see Appendix B). These gratings vary slightly in size. The grating blank for the largest one is approximately eight and three quarter inches wide by six and a half inches high by one and three-eighth inches thick. The grating holder consists of a steel base and an aluminum frame, Figure 19. The grating slides into the frame and is held in place by four padded aluminum fingers which protrude slightly over the grating face. A handle is provided on the top of the grating holder for convenience in handling.

The grating holder stands on a tripod consisting of three adjustable legs. These legs screw into the base and provide the adjustment necessary to align the grating. They are cone shaped on the bottom and have a knurled section so that they may be adjusted by hand. The cone shaped section of the legs fits into grooves in the grating table to provide positive positioning, and the grating mount is fastened in place by a screw which fits through its base and screws into the grating table. Grooves are provided in the grating table for mounting two gratings back to back. Thus two gratings may be brought into play without opening the vacuum tank.

The gratings are stored in grating cabinets to protect them from dust and other elements which might reduce their efficiency. Before placing in the cabinets a grating holder is screwed to a wooden base which protects the cone shaped legs.

The Grating Drives

Two drives are provided for rotation of the gratings about a vertical axis. The first of these drives, called the positioning

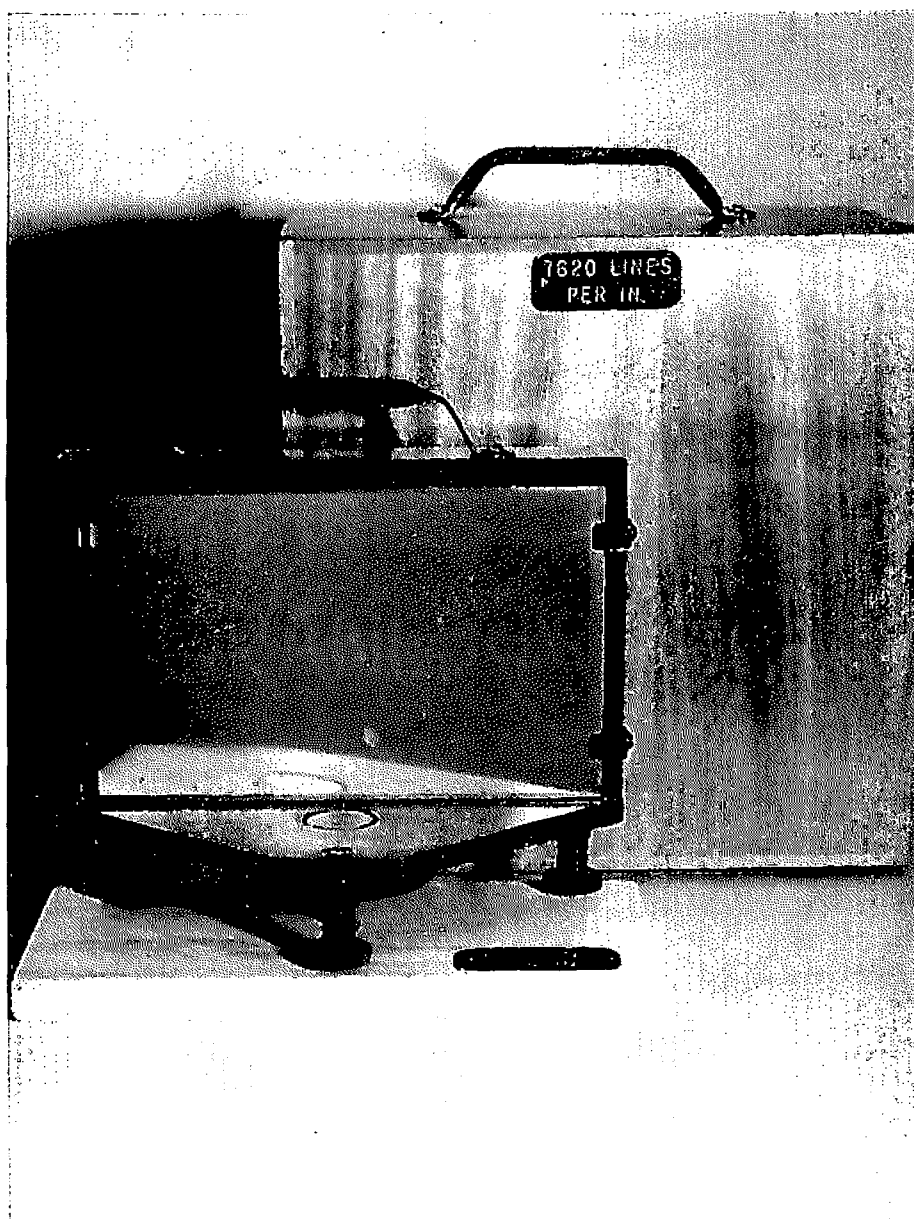


Figure 19. Grating mount and cabinet

drive, provides rotation through 360 degrees by means of a worm gear attached directly to the double cone grating spindle. The second drive, called the scanning drive, provides rotation through about sixteen degrees by means of a long drive arm activated by a precision screw and nut assembly. Both drives rotate the grating spindle, and the grating angle is obtained by adding the angular displacements of the two drives with respect to central image.

The spindle which the drives activate is a double cone unit constructed from a high quality tool steel. Figure 20 is an exploded view of the spindle assembly. The upper and lower female cones are made of unhardened steel while the double male cone is hardened. All cone surfaces are ground and lapped to obtain a run-out of less than 2×10^{-5} radians.

The axis of this lower cone determines the axis of rotation of the gratings. The lower section of the spindle fits through a hole in the spectrometer table and its axis is made perpendicular to the table by placing shims under the flange. It is held in place by four bolts which screw into the flange.

The lower section of the double male cone is relieved so that only the upper and lower ends bear against the lower female cone. These two bearing surfaces as well as the bearing surface of the upper male cone are provided with grease grooves to distribute the lubricant over the mating surfaces. (See Appendix C for lubrication requirements.) The flange between the upper and lower male cones provides an effective seal to prevent dust from getting to the bearing surfaces. The shaft on the upper end of the double male cone carries the grating

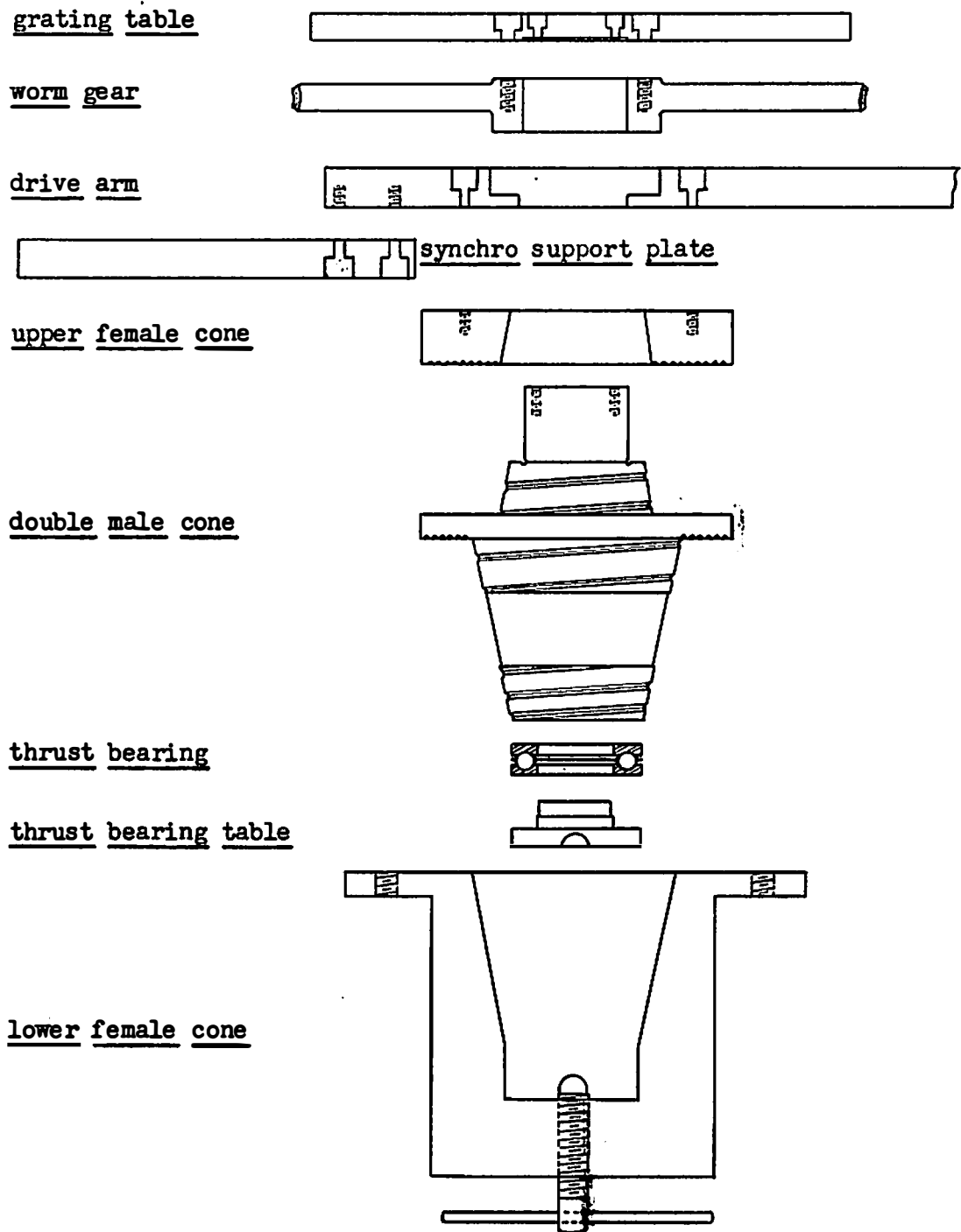


Figure 20. Exploded view of the grating spindle assembly

table and the special precision worm gear for the positioning drive. The thrust bearing and thrust bearing table carry the weight of the rest of the assembly, reduce the friction, and prevent the cones from seizing. The thrust bearing is positioned by a ball and socket joint and may be adjusted by means of the ball screw so that it carries the weight without impairing the accuracy of the cone bearing.

The long drive arm is screwed directly to the upper female cone, and the back end of the arm carries the positioning drive synchro repeater, the reduction gears, and the worm which drives the worm gear, Figure 21. The special precision worm gear has 360 teeth and the reduction gears have a ten to one ratio. The synchro repeater is driven by a synchro transmitter which is located in one of the relay racks, and the speed is controlled by a two speed transmission powered by a one seventy-fifth horsepower reversible synchronous motor. The synchro transmitter also drives a second synchro repeater which turns an angle counter located on the control panel. A block diagram of the system is shown in Figure 22.

The maximum recommended speed for the synchros is 300 rpm, and this was chosen as the top speed for the transmission. Table I gives the knob position, the gear ratios, synchro speeds and grating speeds for the positioning drive. The speed is changed by a gear shift knob on the front of the positioning drive panel, Figure 23, and an idler knob is provided to aid in engaging the gears.

On the left of the positioning drive panel is a power failure relay which turns off the power to the drive systems if the power fails. This relay prevents the drive systems from running when the

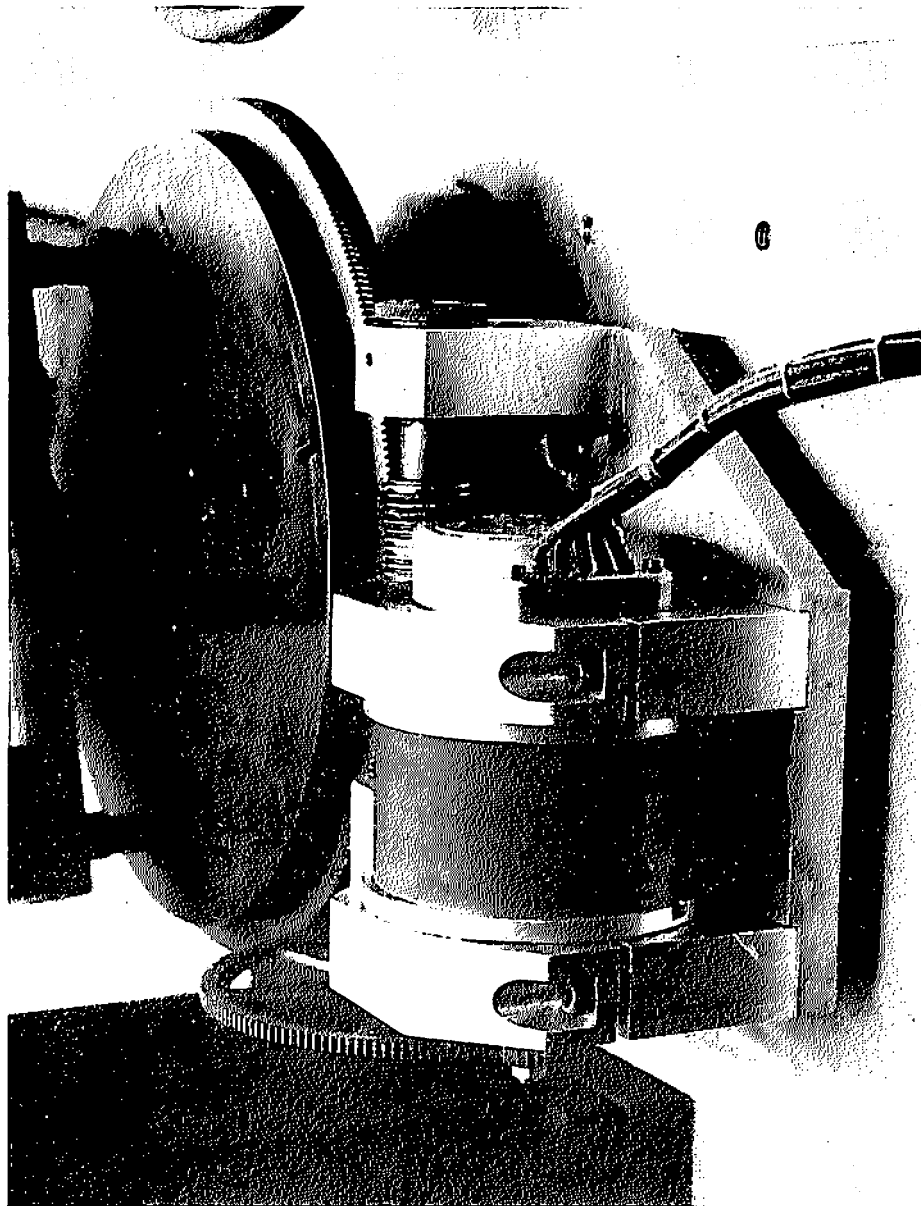


Figure 21. Synchro repeater and gears for the positioning drive

TABLE I

POSITIONING DRIVE DATA

Shift Knob Position	Gear Ratio	Synchro Speed	Grating Speed
1	6:1	300 RPM	30° per minute
2	30:1	60 RPM	6° per minute

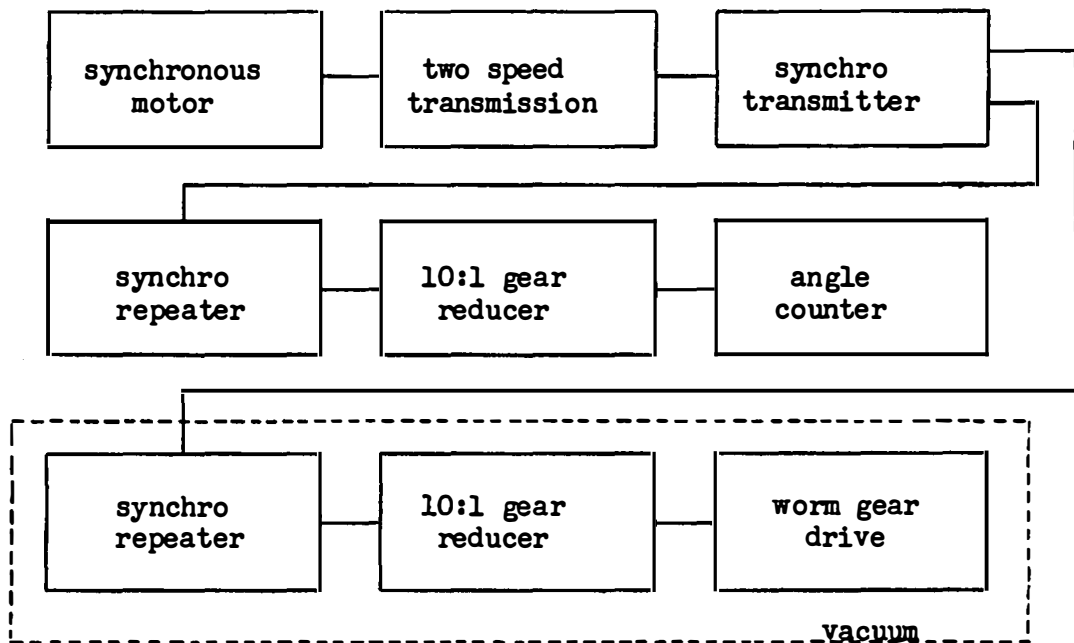


Figure 22. Block diagram of positioning drive

power comes back on and the power failure lamp indicates to the operator that the synchros may be out of phase. This out of phase condition will result if the power fails while the drive is running, because the synchro repeater and synchro transmitter do not come to rest in the same length of time unless they are electrically coupled. If power failure occurs the relay must be reset and the synchros resynchronized.

Figure 24 is a top view of the positioning drive panel showing the synchronous motor, synchro transmitter and transmission with cover removed.

The switches and angle counter system are located on the control panel along with those for the scanning drive, Figure 25. The switches are provided with a mechanical interlock to make sure that the power

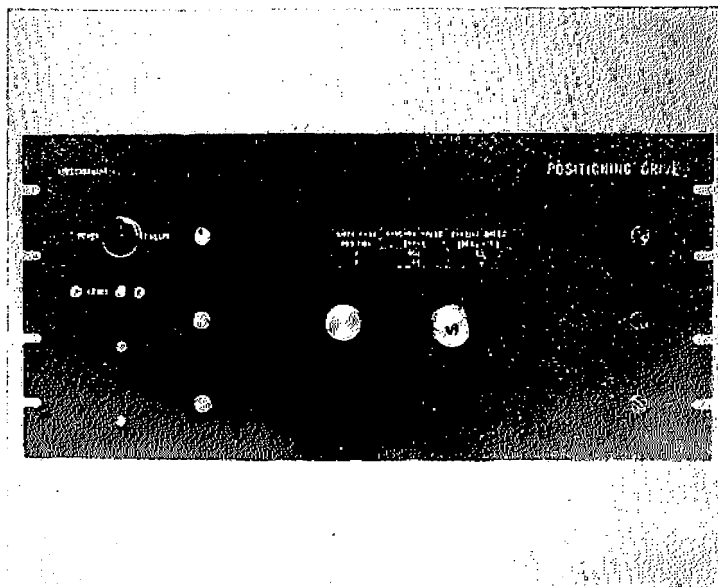


Figure 23. Front view of positioning drive panel

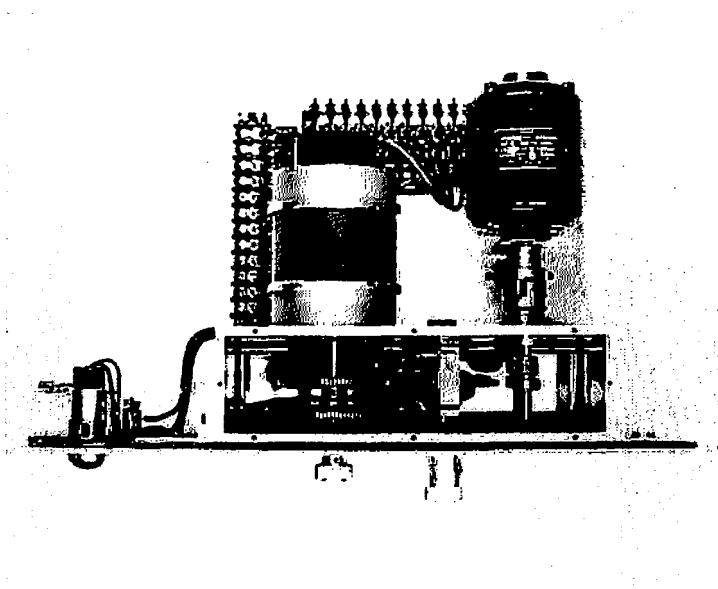


Figure 24. Top view of positioning drive panel

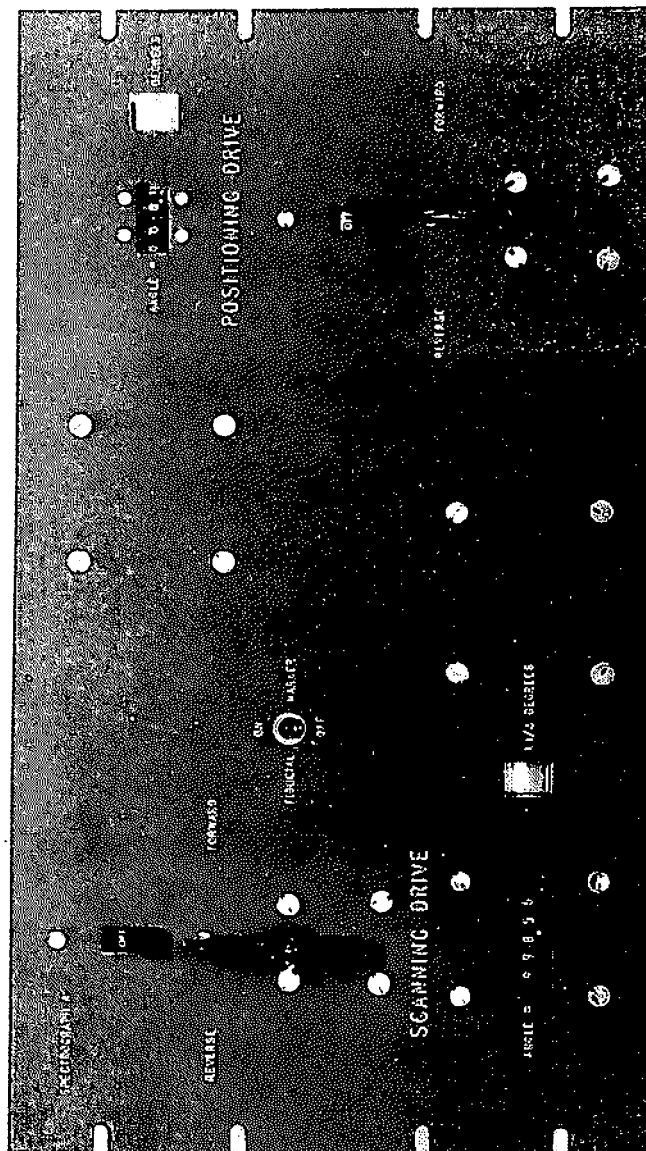


Figure 25. Front view of grating drive control panel

to the synchros is turned on before the synchronous motor is started and to make sure the synchronous motor is turned off before the synchros are turned off. This prevents the synchros from getting out of phase. The wiring diagram of the positioning drive system is given in Figure 26.

The scanning drive, which is slower and smoother than the positioning drive, will rotate the grating through 16.5 degrees at any one of twelve speeds from half a degree per hour to sixty degrees per hour. The drive consists of a long drive arm attached to the upper female cone of the double grating spindle, a precision screw and nut assembly, and a steel tape which connects the end of the long drive arm to the nut, Figure 27.

The long drive arm was machined from a piece of three quarter inch steel plate ten inches wide. The arm is ruggedly constructed to prevent it from flexing when slight variations occur in the amount of friction present in the spindle. The outer end of the arm is the arc of a circle of radius 33.836 inches having its center at the center of rotation of the spindle. The weight of the arm is supported on a pair of casters which ride on a ground steel plate.

Attached to one end of the arc is a steel tape which wraps around a part of the arc and then comes off tangentially to the precision screw and nut assembly. When the scanning drive is running in the forward direction the nut travels along the screw pulling the tape which comes off tangentially to the end of the drive arm. This provides a smooth constant speed drive which does not have the periodic variations inherent in a worm gear drive. When the drive is running

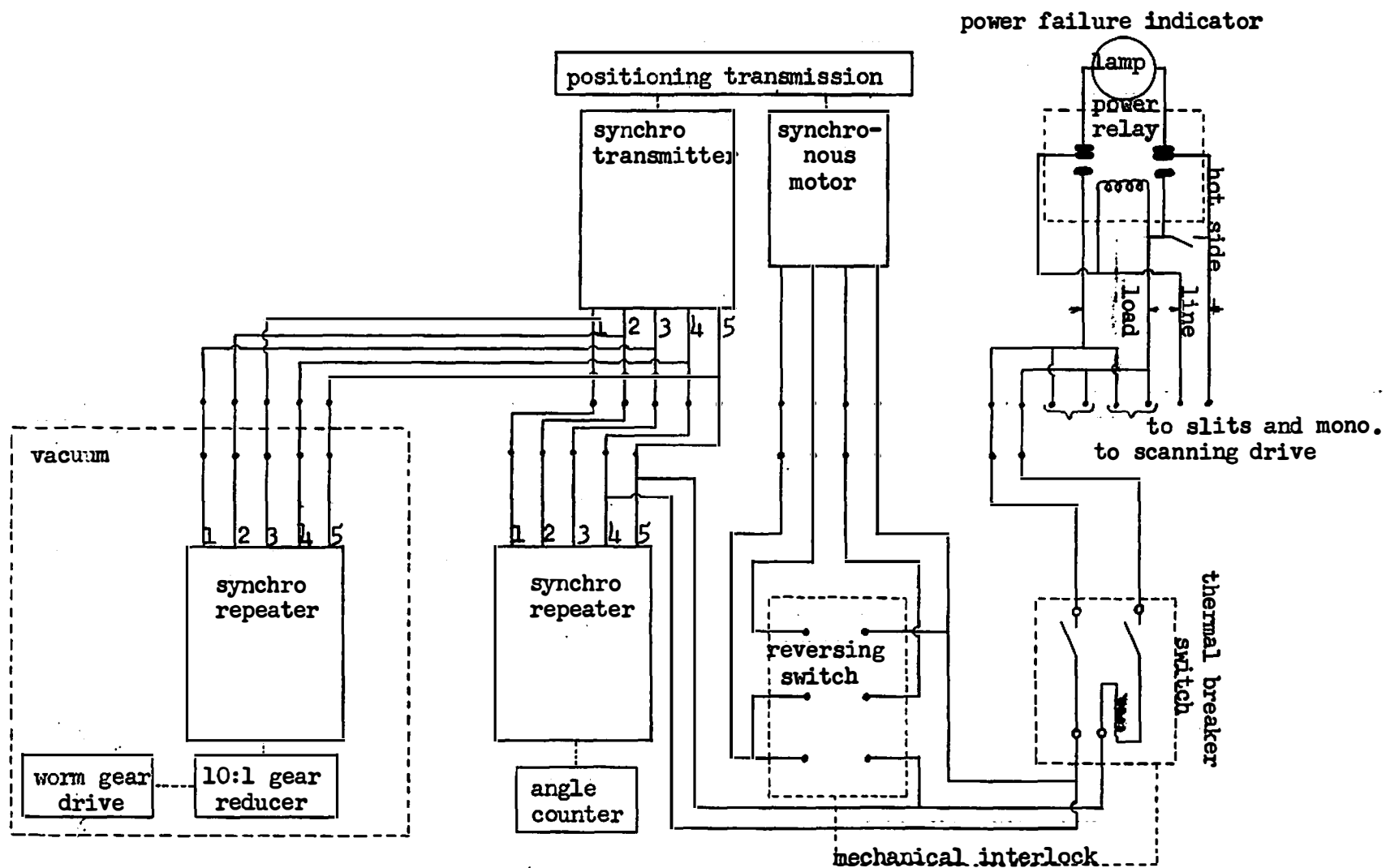


Figure 26. Wiring diagram of the positioning drive system

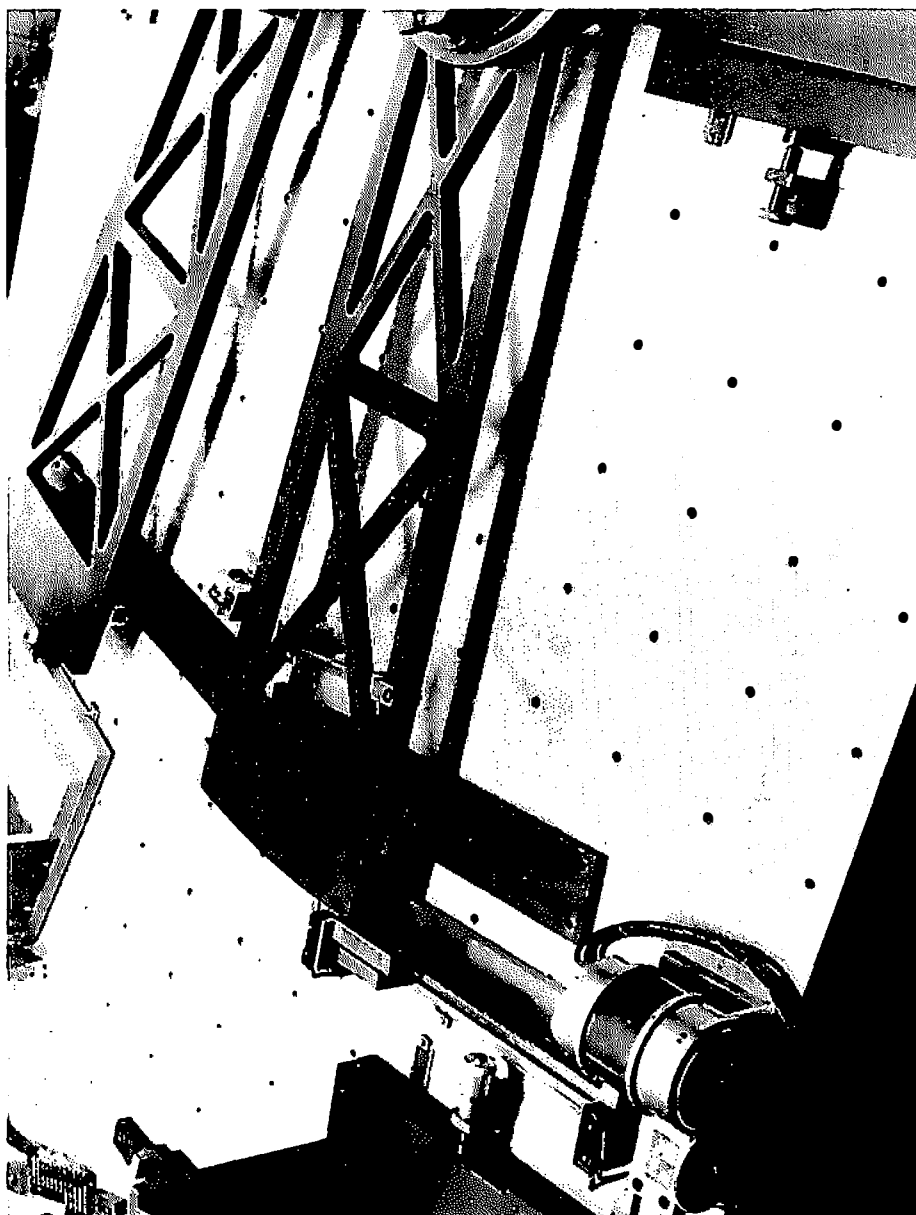


Figure 27. Long drive arm and precision screw and nut assembly

in the opposite direction the tape is held tight by a rope which runs over a pulley to a counter weight beneath the spectrometer table.

The precision screw is mounted in angular contact bearings and is driven by a synchro repeater coupled through a 20:1 speed reducer mounted in one end of the drive screw assembly. The nut rides back and forth on the screw and is guided by a keyway which prevents it from rotating. The speed of the synchro repeater is controlled by the synchro transmitter connected to the scanning drive transmission mounted in one of the relay racks.

The scanning transmission is powered by a one seventy-fifth horsepower reversible synchronous motor, and it is possible to drive the synchro transmitter at any one of twelve speeds by properly setting the four gear shift knobs. The synchro transmitter also drives a second synchro repeater which turns a counter located on the left side of the control panel, Figure 25. Figure 28 is a block diagram of the scanning drive.

The maximum synchro speed for this drive was also chosen as 300 rpm. Table II gives the knob positions, synchro speeds and grating speeds for the scanning drive. The speed is changed by the four gear shift knobs (A, B, C, and D) on the front of the scanning drive panel, Figure 29. Two idler knobs are also provided to aid in engaging the gears. Figure 30 is a top view of the scanning drive panel showing the synchronous motor, synchro transmitter and transmission with cover removed.

The switches and counter system are located on the left of the control panel, Figure 25. And, as in the case of the positioning

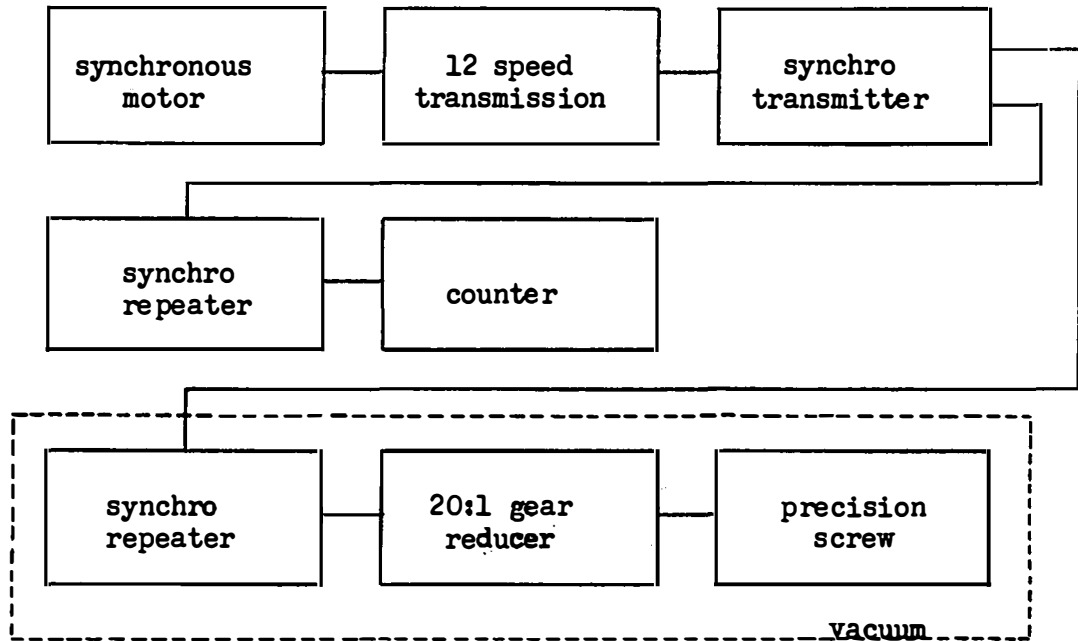


Figure 28. Block diagram of scanning drive

drive, the switches for the scanning drive are provided with a mechanical interlock to make sure that the power to the synchros is turned on before the synchronous motor is started and to make sure the synchronous motor is turned off before the synchros are turned off. The wiring diagram for the scanning drive system is given in Figure 31.

The angle at which the scanning drive is set is obtained by dividing the scanning drive counter reading by three, and the angle at which the positioning drive is set is read directly from the positioning drive counter. The positioning drive angle may be read with an accuracy of about ± 0.001 degrees, while the scanning drive angle may be read with an accuracy of better than ± 0.0001 degrees. The absolute accuracy of the instrument, however, is not dependent on the

TABLE II
SCANNING DRIVE DATA

Shift Knob Position				Synchro Speed (RPM)	Grating Speed (degrees per hour)
A	B	C	D		
1	1	2	1	2 $\frac{1}{2}$	1 $\frac{1}{2}$
1	1	2	2	5	1
1	2	2	1	5	1
1	2	2	2	10	2
2	1	2	1	12 $\frac{1}{2}$	2 $\frac{1}{2}$
1	1	1	1	15	3
2	2	2	1	25	5
2	1	2	2	25	5
1	2	1	1	30	6
1	1	1	2	30	6
2	2	2	2	50	10
1	2	1	2	60	12
2	1	1	1	75	15
2	2	1	1	150	30
2	1	1	2	150	30
2	2	1	2	300	60

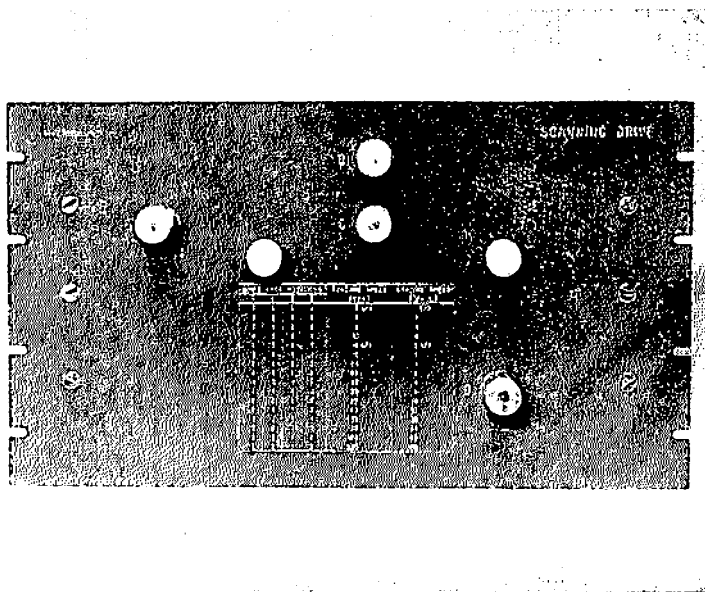


Figure 29. Front view of scanning drive panel

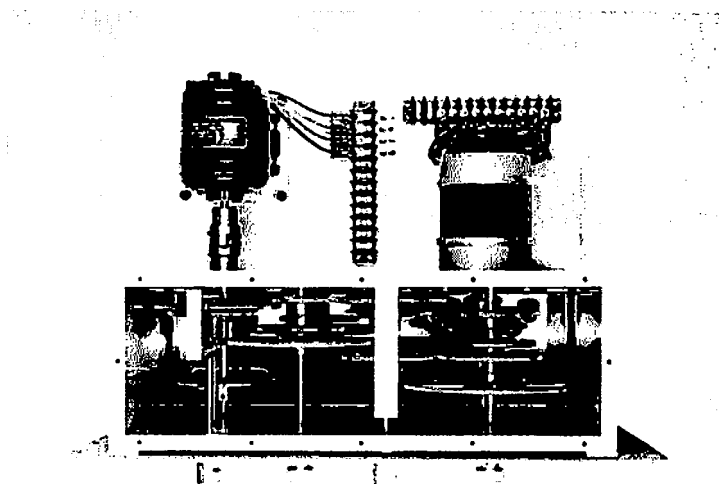


Figure 30. Top view of scanning drive panel
with transmission cover removed

accuracy of the drives but depends only on the accuracy with which the standard line and the Fabry-Perot etalon spacing are known.

The Slit System

The slit jaws S_2 and S_3 , Figure 15, for the grating monochromator are mounted on a modified Perkin-Elmer slit spindle assembly². The slit spindles have been cut down and moved closer together so that both slits can "see" the paraboloidal mirror M_{10} through the hole in M_{11} . The slit jaws for S_2 are curved in accordance with the discussion on slit curvature, page 21; and the slit jaws for S_3 are straight. Both slits are one and a half inches long.

The slit spindles (seen at the right of Figure 32) are coupled together so that both slits are adjusted simultaneously and both have the same width. The slit width is adjusted by positioning the slit control arm (not shown) with a screw and nut assembly which is driven through a pair of bevel gears by a synchro repeater. The synchro repeater is in turn driven by a synchro transmitter connected to a twenty-five turn Duodial. The Duodial is located on the slit control panel, Figure 13 i), and the linkage is adjusted so that the Duodial reads directly in microns of slit width. Figure 33 is a block diagram of the slit control system.

The slit spindles are mounted on a plate connected to the back of the mirror mount for M_{11} as shown in Figure 32. This same plate also carries the detector and detector optics, and it is provided

²Drawing No. 021-0446, (The Perkin-Elmer Corp., Norwalk, Conn.)

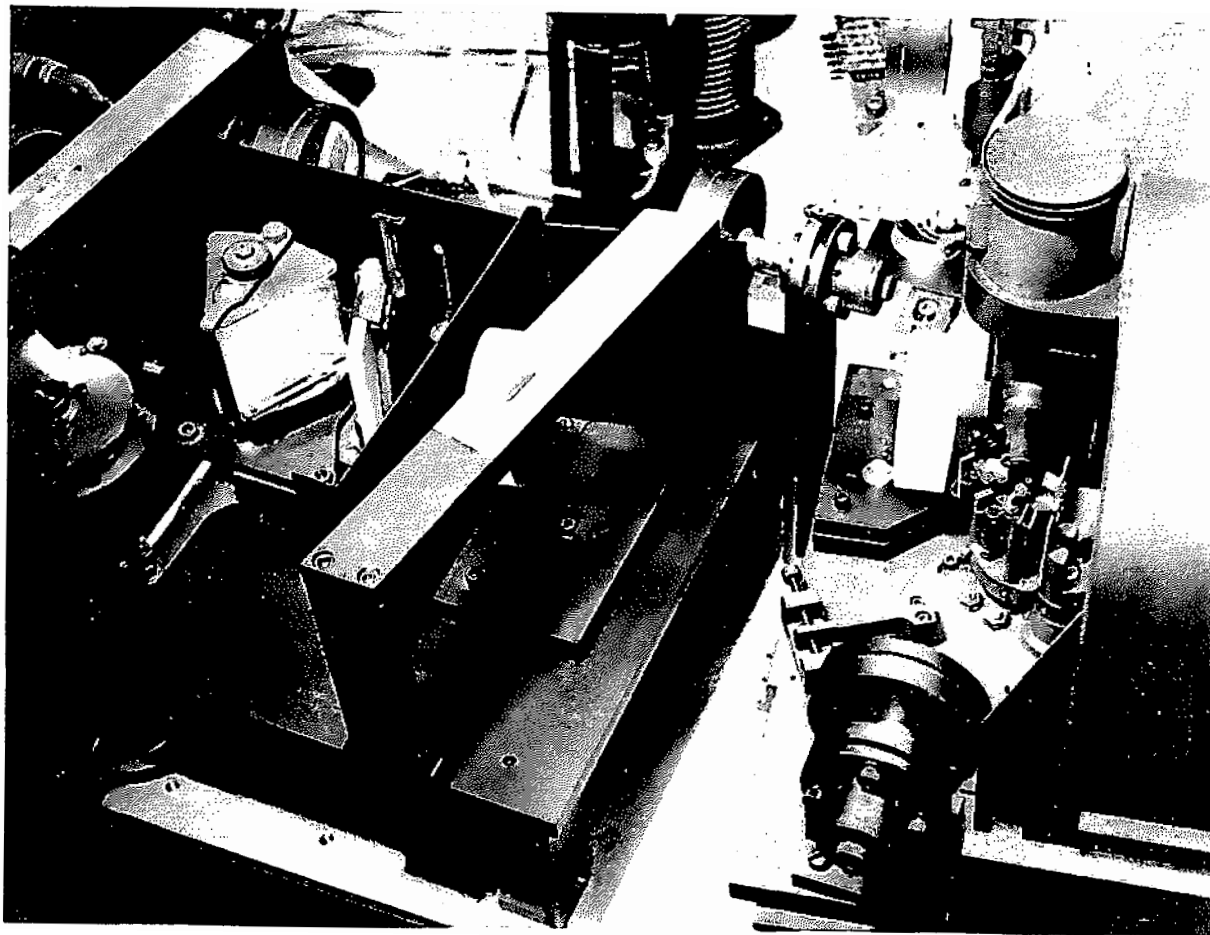


Figure 32. Prism monochromator section showing the slits for the grating monochromator

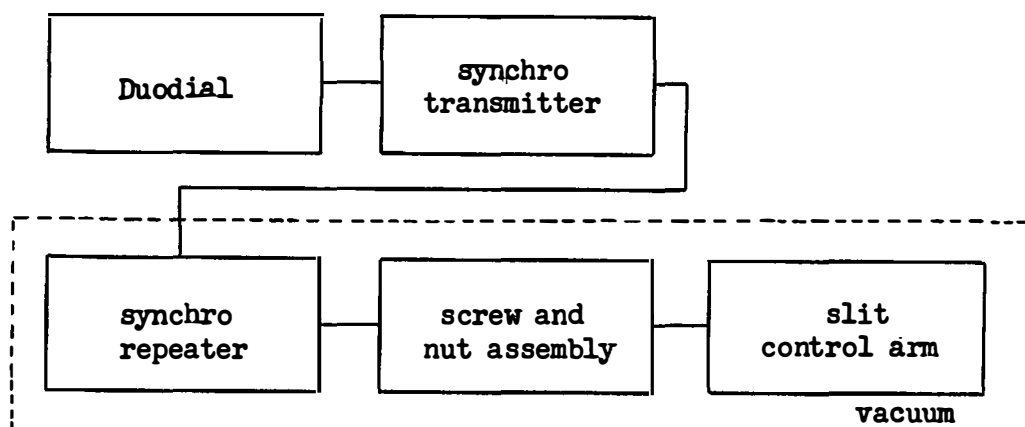


Figure 33. Block diagram of the slit control system

with appropriate adjustments for aligning the slits.

The Source Optics, Prism Monochromator, and Detector Optics

When infrared absorption spectra are being observed, the radiation which enters the grating monochromator comes from a Nernst glower, L_1 , which supplies a continuous spectrum of infrared frequencies. Before entering the grating monochromator the light is dispersed by a prism monochromator, Figure 32. The optical scheme for getting the radiation to the entrance slit, S_2 , of the grating monochromator is shown in Figure 34. L_2 is a second source such as a krypton arc, and it is used as a frequency standard in the Fabry-Perot calibration system. Either L_1 or L_2 may be used as the source by rotating the spherical mirror M_1 .

The Optical Path

The radiation from the source is intercepted by the spherical mirror M_1 and brought to a focus at f_1 , Figure 34. It then strikes the spherical mirror M_2 and is brought to a second focus f_2 in the center of the sample cell area. After passing through the sample cell it is brought to a focus by the spherical mirror M_3 on the entrance slit S_1 of the prism monochromator after being deflected by the plane mirror M_4 . After passing through the entrance slit S_1 , the radiation is deflected by the plane mirror M_5 to the paraboloidal mirror M_6 , which collimates the beam and sends it through the prism P. The dispersed beam is then reflected back through the prism by the Littrow mirror M_7 and dispersed a second time. The radiation is then brought to a focus in a spectrum by M_6 at the chopper C. After leaving the prism monochromator the spectrum is brought to a focus on the entrance slit S_2 of the grating monochromator by the two paraboloidal mirrors M_8 and M_9 . Upon traversing the grating monochromator, the radiation which passes through the exit slit S_3 is deflected by the plane mirror M_{12} and is brought to a focus on the detector by the ellipsoidal mirror M_{13} .

The Mirror Holders

The mirror holders for mirrors M_1 , M_2 , M_3 , and M_{13} are similar to those used by the Perkin-Elmer Corporation³ in their prism spectrographs. These mirror mounts have adjustments for focusing and for

³Drawing No. 098-0027, (The Perkin-Elmer Corp., Norwalk, Conn.)

rotation about a vertical and a horizontal axis.

The mirror holder for M_1 has the additional feature that it may be rotated about a vertical axis from outside the vacuum by means of the synchro system shown in the block diagram, Figure 35. The mirror mount for M_1 is shown in Figure 36. The gears which couple

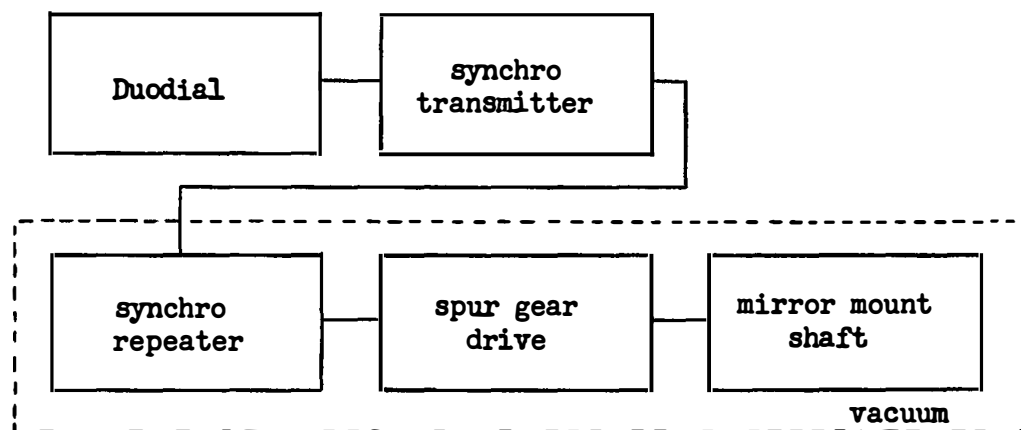


Figure 35. Block diagram of mirror rotating system

the synchro repeater to the mirror mount shaft are located in the base of the mirror mount. The mirror is positioned by means of the source selector dial on the control panel, Figure 13 d).

The Sample Cell Area

The sample cell area in the present system will accommodate cells up to twenty centimeters in length. If it is necessary to use a longer absorbing path the optics may be repositioned to give a

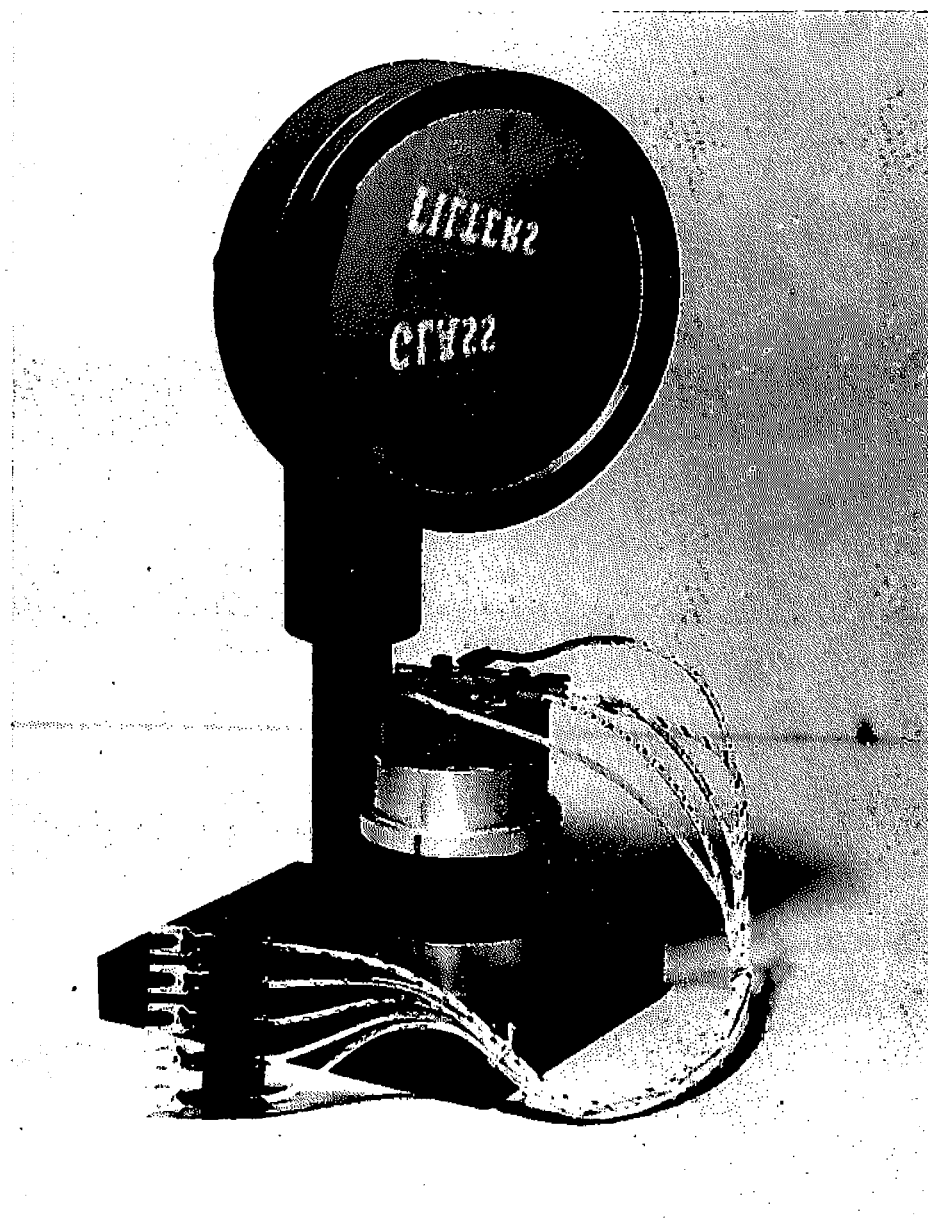


Figure 36. Mirror mount for M_1

parallel beam through the sample cell area. When such a parallel beam of light is used the image at S_1 is reduced in size and intensity because light coming from the ends of the Nernst glower diverges from the optic axis and is not intercepted by the condensing mirror. The amount of light lost because of this effect depends on the separation of the collimating and condensing mirrors. As the distance between these mirrors is increased the amount of light which spills over the condensing mirror is also increased, thus reducing the size and intensity of the image at S_1 . This type of optical arrangement will, however, allow cells having lengths up to forty centimeters to be used.

If longer path lengths are needed, a multiple reflection cell will be required. It has been proposed that such a multiple reflection cell having a f-number matching that of the spectrograph (f:5) be mounted underneath the spectrometer table. In order to get light to this cell, two holes have been cut in the front end of the table.

The Prism Monochromator

The prism monochromator, Figure 32, is a Perkin-Elmer basic interchange unit⁴ with the slit servo system removed. The unit is equipped with a rock salt prism and a linear wave number cam which drives the Littrow mirror M_7 . The cam is driven by means of a worm and worm gear coupled to a synchro repeater. The scheme for adjusting the prism monochromator is shown in the block diagram, Figure 37.

⁴Drawing No. 021-0710, (The Perkin-Elmer Corp., Norwalk, Conn.)

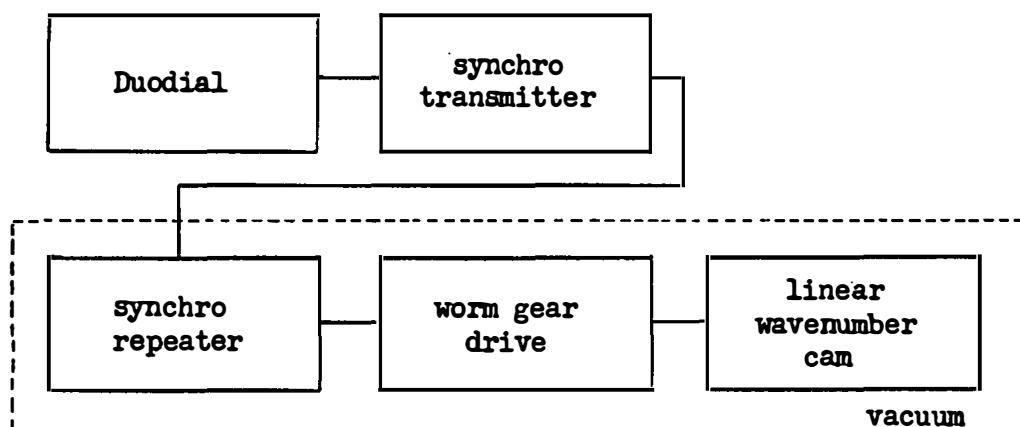


Figure 37. Block diagram of prism monochromator drive

The monochromator setting is presently adjusted manually by the monochromator dial on the control panel, Figure 13 i); however, it would not be difficult to drive the prism monochromator so that it would follow the grating monochromator. (The instructions for setting the prism monochromator are given in Appendix D.)

At present a wide entrance slit S_1 is used so that prism monochromator adjustments are infrequent. This is a fixed slit cut in a brass plate which slides into a slit plate holder. Two slits of different widths are available. A narrow slit having a width of about 0.003 inches is used in focusing the monochromator, while a slit having a width of 0.065 inches is normally used in running the instrument. Both of these slits have a radius of curvature of 4.25 inches. This slit curvature is such that it over compensates for the

image curvature caused by the prism monochromator so that the image falling on S_2 matches the curvature of that slit.

There is no exit slit for the prism monochromator, because one wishes to have a fairly broad band of frequencies falling on the entrance slit of the grating monochromator to reduce the need for frequent prism monochromator adjustments.

The Chopper

A light chopper C has been placed at the focus where the exit slit of the prism monochromator would normally be. This is a Perkin-Elmer thirteen cycle chopper⁵ for use with their Model 107 amplifier⁶. The chopper assembly is mounted below the base of the prism monochromator, and the light interrupter projects through the base and into the light path. On the lower end of the chopper shaft are three cams which activate the breaker rectifier used in the amplification system. The shaft is belt driven by a motor mounted on the chopper assembly beneath the prism monochromator table.

Mirrors M_8 and M_9

After the light is chopped it is focused on the entrance slit S_2 of the grating monochromator by the two mirrors M_8 and M_9 . These are Perkin-Elmer stem-mounted eighteen degree off-axis paraboloidal mirrors⁷. They are held in kinematic mounts⁸ like those used by

⁵Drawing No. 099-0026, (The Perkin-Elmer Corp., Norwalk, Conn.)

⁶"Instruction Manual, Vol. 3A", (The Perkin-Elmer Corp., Norwalk, Conn., 1953), p. 14.

⁷Drawing No. 095-0041, (The Perkin-Elmer Corp., Norwalk, Conn.)

⁸Drawing No. 098-0040, (The Perkin-Elmer Corp., Norwalk, Conn.)

Perkin-Elmer for this purpose.

Paraboloidal mirrors are used here to prevent distortion of the image at the entrance slit of the grating monochromator. This is to insure that a maximum amount of energy will pass through S_2 .

The Detector Optics

The light which comes through the exit slit of the grating monochromator S_3 is reflected by the plane mirror M_{12} and focused on the detector by the ellipsoidal mirror M_{13} . This ellipsoidal mirror reduces the size of the image to 0.177 times its original size so that all of the energy will fall on the sensitive element of the detector.

These detector optics are adequate for detectors such as thermocouples and PbS cells, where the size of the detector unit is small. If larger units such as Golay cells or cooled Dewar type PbS or PbTe cells are to be used, the detector optics will have to be modified. It is, however, quite probable that special cooled detectors may be built to fit into the present system.

The Fabry-Perot Optical System

The Fabry-Perot system is mounted above the prism monochromator, Figure 38, and the interference pattern is projected onto the top of the entrance slit of the grating monochromator, S_2 . The light from the Fabry-Perot pattern which passes through S_2 is dispersed by the grating monochromator and that portion having a wavelength $\lambda_m = m\lambda$ emerges from the bottom of the exit slit, S_3 , and is focused on a photomultiplier. Orders other than m are eliminated by the use of

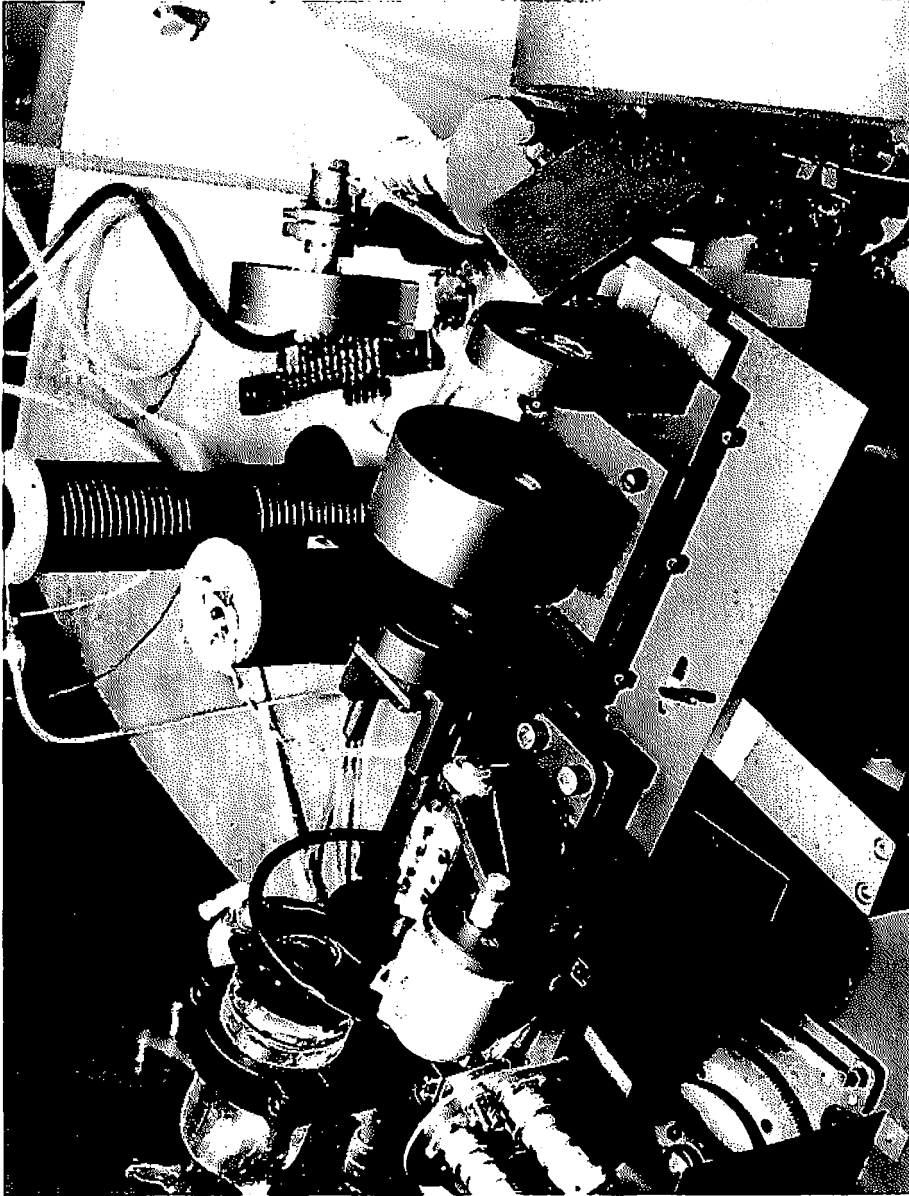


Figure 38. Fabry-Perot system

appropriate filters.

The optical path for the Fabry-Perot etalon is shown in Figure 39. Figure 39a is a side view of the premonochromator optics. The light from a one hundred watt zirconium arc⁷ L_3 , is interrupted at thirteen cycles per second by the chopper C, passes through a group of filters, F, and is collimated by the lens L_1 . The parallel light from L_1 passes through the Fabry-Perot etalon, E, and the interference pattern is imaged on the top of the entrance slit, S_2 , by the lens L_2 after being brought down to the spectrograph level by the two plane mirrors M_{14} and M_{15} . After traversing the grating monochromator the radiation which passes through the exit slit S_3 (Figure 39b) is deflected by the plane mirror M_{16} and focused on the photomultiplier, P, by the lens L_3 .

The filters used in this system are Corning Glass Color Filters. Normally two filters are used to provide a sufficiently narrow band of frequencies so that only light of order m will get through the grating monochromator. (For filter data and details for operating the Fabry-Perot system see Appendix E.) The etalon mount is similar to that described by Schreiber⁸. The lenses L_1 , L_2 , and L_3 are uncoated glass achromats. These glass lenses may be used here because

⁷This is a Sylvania type C100 lamp which has had a glass cooling jacket blown around it. The lamp also has a sapphire window so that it may be used as an infrared source.

⁸Paul Schreiber, "Use of Fabry-Perot Interferometer for Wavelength Calibrations in the Infrared" (Unpublished M.S. thesis, Department of Physics, Ohio State University, September 1956).

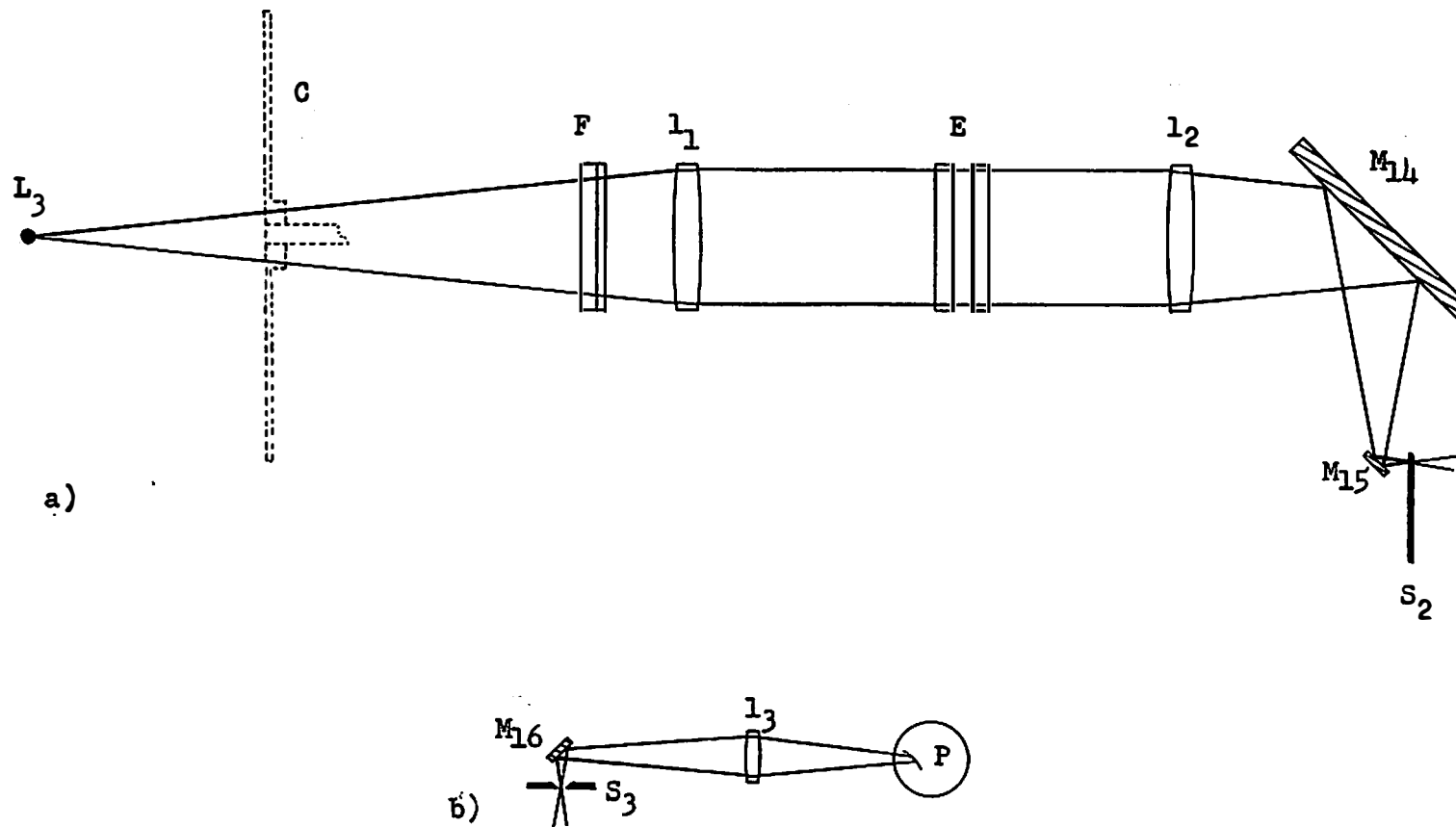


Figure 39. Optical path of the Fabry-Perot system
 a) side view of premonochromator optics
 b) top view of post monochromator optics

the light used in the Fabry-Perot calibrating system falls in the visible region of the spectrum and is not absorbed by glass. The plates used in the etalon are aluminum coated quartz flats having a transmission of about six per cent. The mirrors M_{14} , M_{15} , and M_{16} are front surface mirrors.

P is an RCA 1P22 photomultiplier tube which is housed in an air tight chamber. This photomultiplier housing is maintained at atmospheric pressure to prevent the high voltage on the tube from arcing across its pins. The housing also shields the sensitive area of the tube from stray light, and the lens L_3 is sealed into the body of the housing and acts as a window.

Power Supplies

Special power supplies are required for the Nernst filament, the zirconium arc, the krypton arc, and the 1P22 photomultiplier tube. These power supplies are mounted in the relay racks outside the vacuum system.

The Nernst glower is an earth oxide filament having an extremely high resistance at room temperature; however, as the glower is heated its resistance decreases to the point where it will carry enough current to maintain its temperature with only a few hundred volts applied across it. When used as an infrared source, the glower is usually operated at a current of one ampere and a voltage which varies from 120 to 200 volts A.C., depending on the condition of the filament.

In order to light the glower, it has been surrounded by a series

of nickel wire heating coils, Figure 40, which raise the temperature of the glower to a point where it will maintain itself. The heating coils are in turn surrounded by a cooling jacket which reduces the amount of heat radiated to the vacuum system.

The power supplies for both the Nernst glower and the heater are built into a single unit, Figure 13 1.). The circuit, Figure 41, is designed so that the glower will light automatically once the heater voltage and current are set. As the glower heats up it draws more and more current, and, when the current reaches 0.1 amperes, the relay, R, is closed turning off the power to the heater and connecting the Nernst glower variac across the filament. The current may then be set at the desired value.

The glower may be lighted at atmospheric pressure or in vacuum, but the heater voltage and current requirements are quite different for different pressures. Table III gives the voltage and current settings for two different pressures. These values must not be exceeded or the heater will be burned out.

When the spectrograph is not in use, the glower is turned down to about 0.3 amperes and allowed to run at this setting. It has been found that the thermal shock of lighting the glower drastically shortens its life, and, therefore, the glower is almost never turned off. The glower heater is provided only for lighting new glowers or for relighting glowers that have gone out due to power failure.

Two zirconium arc power supplies, Figure 13 a) and b), are provided in case one wishes to use this type of source for both the

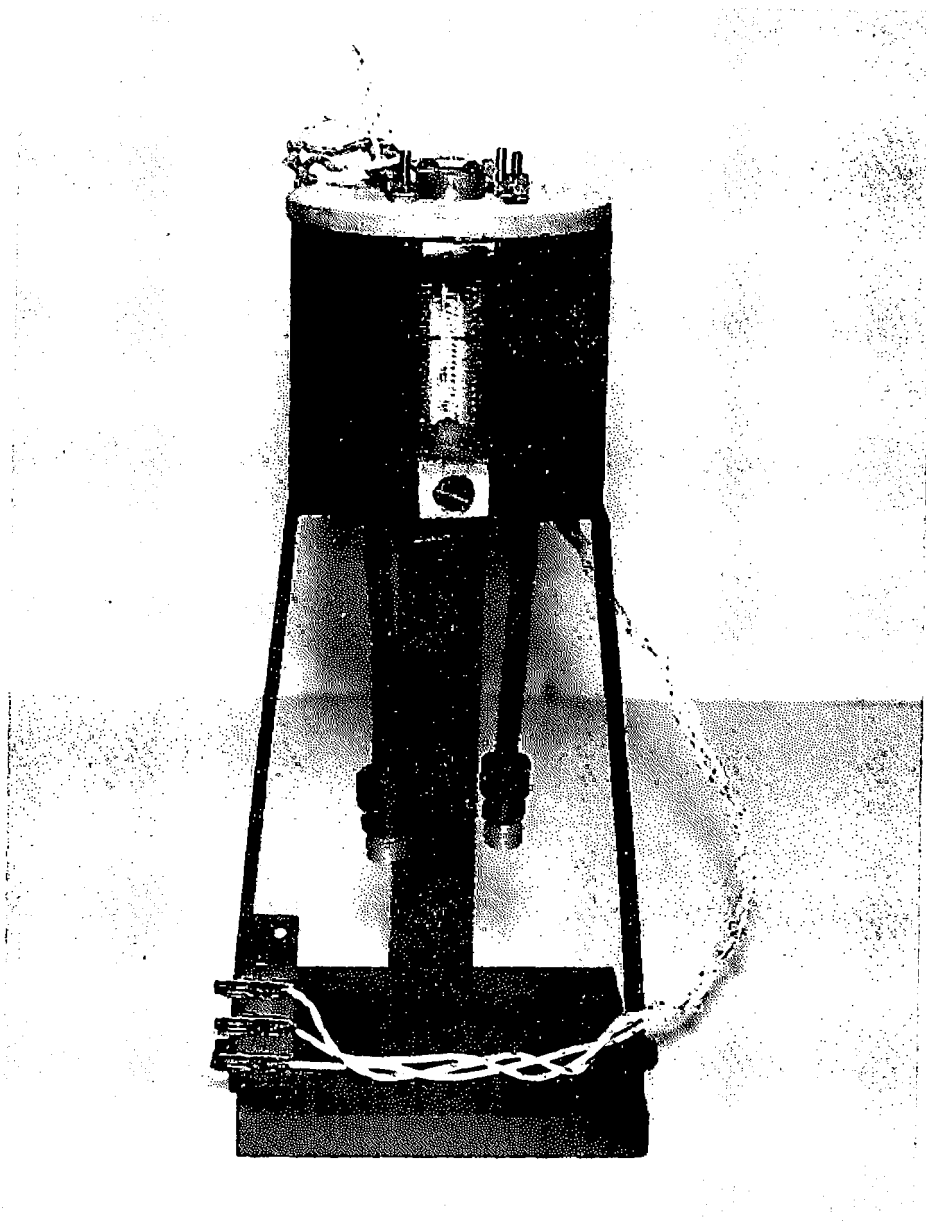


Figure 40. Nernst glower, heater, and cooling jacket

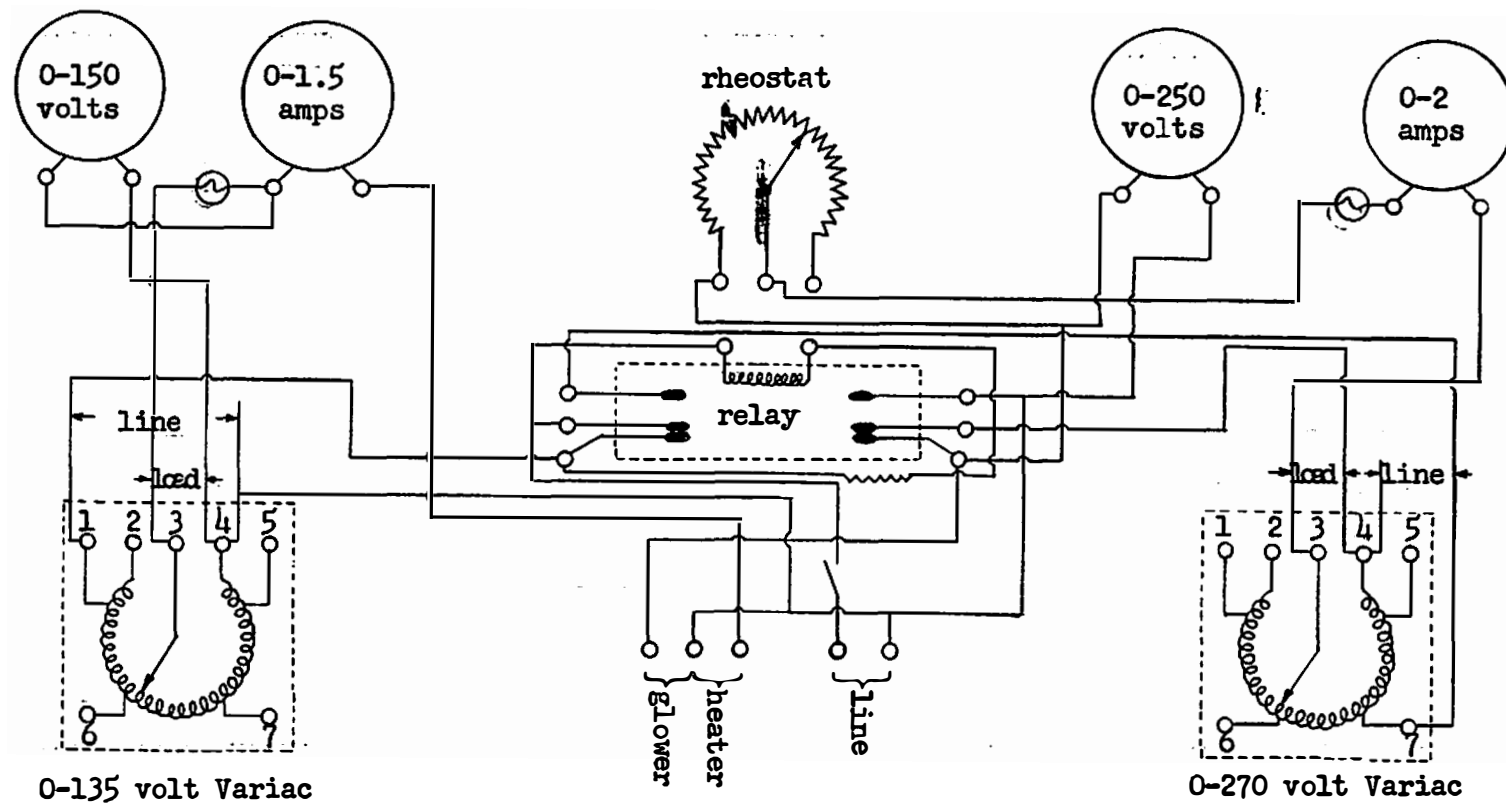


Figure 1. Circuit diagram for Nernst glower and heater power supply

TABLE III

HEATER CURRENT AND VOLTAGE

Pressure	Voltage	Current
1 atmosphere	115 volts	7.2 amperes
300 microns	62 volts	4.7 amperes

Fabry-Perot and infrared systems. The C100 zirconium arc lamp operates on direct current at 15.4 volts and 6.25 amperes. The circuit diagram of the power supply is given in Figure 42.

The switch VS in the power supply circuit, Figure 42, is a Gates Vacuum Switch Assembly No. 4376-A which starts the lamp automatically when the power is turned on. When the main switch is turned on, direct current flows through the inductor, C, the resistor, R, and the vacuum switch. A magnetic field is generated across the air gap in the iron core of the inductor, C, opening the vacuum switch and interrupting the current. When the current is interrupted, an inductive pulse, generated across C, breaks down the gap in the lamp and the lamp becomes operative. And the lamp current flowing through C holds the vacuum switch open. The relay is used to protect the voltmeter from the high voltage generated by the inductor and vacuum switch. When the current starts to flow in the arc lamp, the relay is activated putting the voltmeter in the circuit.

The power supply for the 100 watt krypton arc⁹, Figure 13 c), has a starting circuit similar to that for the zirconium arc, except that it operates on alternating current. The krypton arc operates on 20 volts A.C. at 5.0 amperes. The circuit diagram for the power supply is shown in Figure 43. After the power is turned on, the lamp is started by depressing the switch S. This removes the voltmeter from the circuit and completes the vacuum switch circuit.

⁹This is a Westinghouse Experimental Spectroscopic Krypton Lamp which has been mounted in a brass tube surrounded by cooling coils.

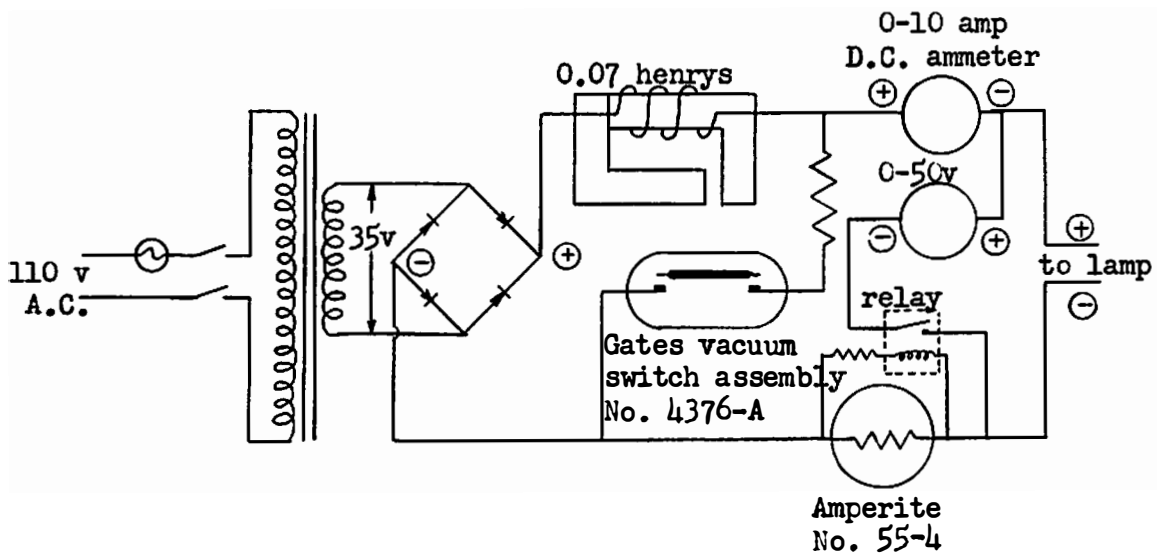


Figure 42. Circuit diagram of zirconium arc power supply

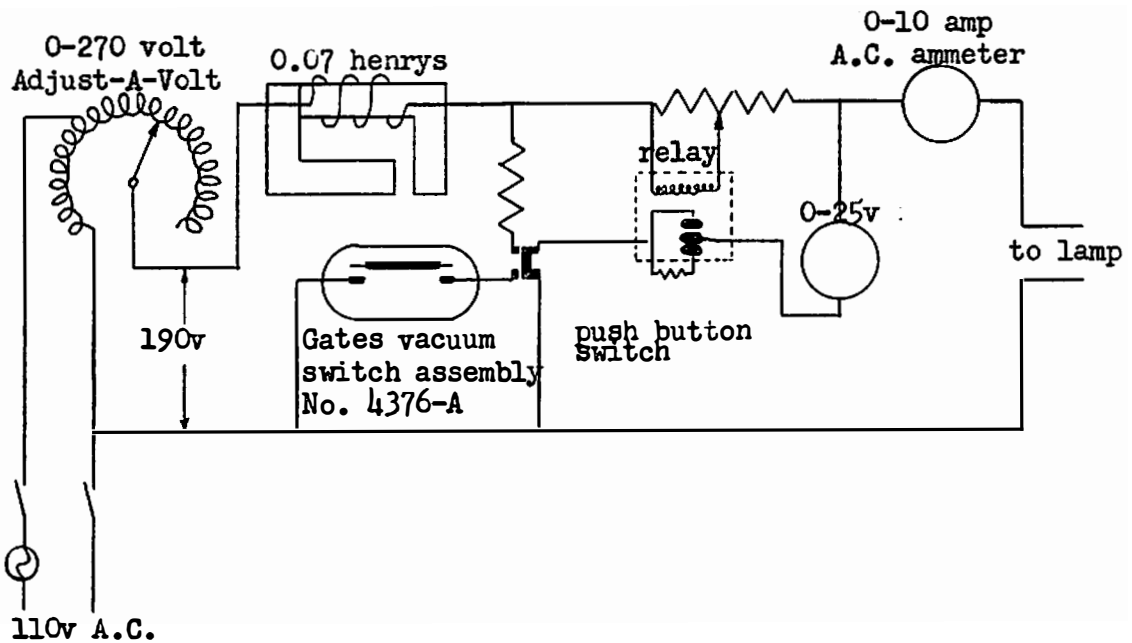


Figure 43. Circuit diagram of krypton arc power supply

Once the lamp starts S is released, and the voltmeter is again in the circuit.

The power supply for the 1P22 photomultiplier, Figure 13 e), is a regulated high voltage supply whose output is continuously variable from 400 to 1500 volts D.C. at 0 to 1 milliamperes. The output voltage varies less than 0.01 per cent of the output voltage per volt change of line voltage and less than one volt with variations of output current from zero to one milliampere. The circuit diagram is given in Figure 44. It is one of the well known voltage regulator circuits used in commercial power supplies¹⁰.

The Amplification and Recording Systems

Both the infrared and Fabry-Perot signals are amplified by the Perkin-Elmer thirteen cycle amplification system¹¹. When a thermocouple is used as the detector, the signal is fed into a preamplifier before going on to the Perkin-Elmer Model 107 amplifier, Figure 13 j). The signals from lead sulfide cells or photomultipliers are fed directly into the Model 107 amplifier. Other types of detectors have not yet been obtained for the instrument; however, when they become available, it may be necessary to build special amplification systems to take full advantage of the peculiar characteristics of

¹⁰"Instruction Manual for Regulated Power Supply Models 710-P and 710-PR", (Furst Electronics Inc., Chicago, Ill.)

¹¹"Instruction Manual, Vol. 3A", (The Perkin-Elmer Corp., Norwalk, Conn., 1953), p. 14.

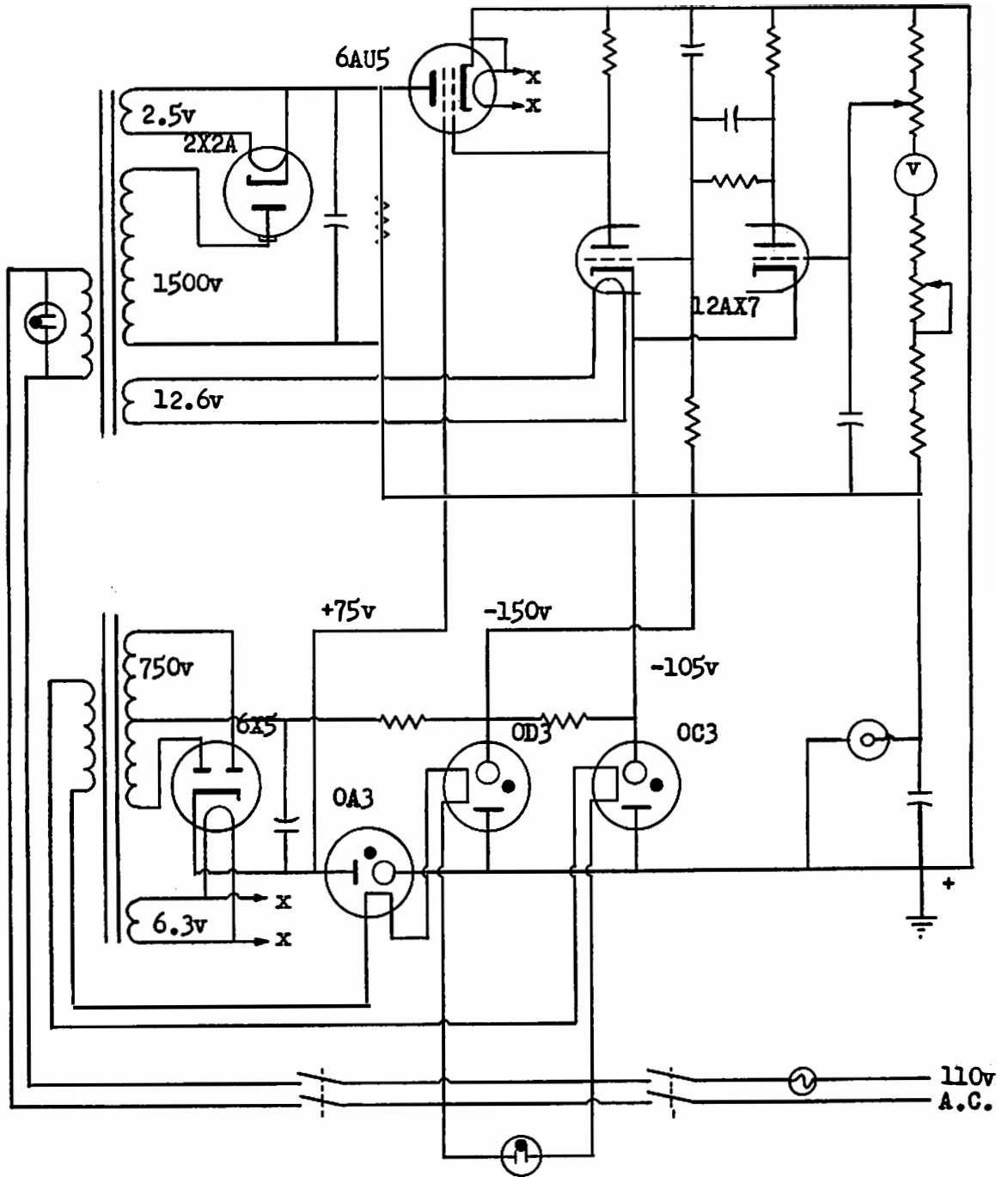


Figure 44. Circuit diagram for photomultiplier power supply

these detectors.

After the signals are amplified they are displayed on a chart by a Leeds and Northrup double pen Speedomax Type G $X_1 - X_2$ recorder¹². The two pens are separated by about one-sixteenth of an inch so that both may travel the full width of the chart paper. The chart paper runs at a speed of thirty inches per hour, and both the infrared signal and the Fabry-Perot signal are recorded at the same time. The two pens carry different colors of ink so that the two signals can be easily identified.

¹²

"Direction Book 77-10-0-9", (Leeds and Northrup Co., Philadelphia, Pa.)

these detectors.

After the signals are amplified they are displayed on a chart by a Leeds and Northrup double pen Speedomax Type G $X_1 - X_2$ recorder¹². The two pens are separated by about one-sixteenth of an inch so that both may travel the full width of the chart paper. The chart paper runs at a speed of thirty inches per hour, and both the infrared signal and the Fabry-Perot signal are recorded at the same time. The two pens carry different colors of ink so that the two signals can be easily identified.

¹²"Direction Book 77-10-0-9", (Leeds and Northrup Co., Philadelphia, Pa.)

CHAPTER IV

PERFORMANCE OF THE SPECTROGRAPH

The Method of Testing

To test the performance of the spectrograph, several well-known absorption bands were recorded and compared with the best data available from other sources. The object of such a comparison was 1) to demonstrate that the resolving power of the instrument is at least as good as that of comparable high-resolution spectrographs, 2) to demonstrate that the vacuum system controls the pressure of atmospheric absorbers allowing more accurate data to be obtained, 3) to demonstrate that the instrument produces substantially better data than the prism-grating spectrograph used by the University of Tennessee Department of Physics since about 1947, and 4) to demonstrate that the Fabry-Perot calibrating system is capable of producing data with an absolute accuracy of the order of a hundredth of a wave number.

To carry out the aims stated above, records were made of four molecular absorption bands as follows:

- 1) Records were made of the 2.7μ water band using a small amount of water vapor in the optical path of the instrument, and these were compared with a similar record made on the high-resolution vacuum-grating spectrograph of The Ohio State University¹.

¹Private communication from K. N. Rao, Department of Physics, The Ohio State University to Dr. A. H. Nielsen dated September 30, 1957.

- 2) A record was made of the 4.25μ carbon dioxide band, and this record was compared with a record of the same region obtained from a non-vacuum type spectrometer².
- 3) A record was made of the ν_3 and $\nu_2 + \nu_4 + \nu_5$ absorption bands of acetylene which overlap in the 3.05μ region, and this record was compared with the best record obtained from the University of Tennessee's older model prism-grating spectrograph³.
- 4) A record was made of the 2.34μ carbon monoxide band and two standard krypton lines⁴ simultaneously with the interference pattern of the Fabry-Perot interferometer, and this record was compared with recent high precision measurements on the same band^{5,6}.

Detailed accounts of these records and their significance are given in the following sections.

The 2.7μ Water Band

Figures 45 a and b and 46 are photographic reproductions of the

²A. H. Nielsen and Y. T. Yao, Phys. Rev. 68, 173 (1945).

³Fred L. Keller, "An Evaluation of the Harmonic and Anharmonic Constants of C_2H_2 from a Re-Investigation of its Infrared Spectrum" (Unpublished Ph.D. thesis, Department of Physics, The University of Tennessee, June 1956), pp. 77-8.

⁴E. K. Plyler, L. R. Blaine, and E. D. Tidwill, J. Res. Nat. Bur. Stand. 55, 279 (1955).

⁵D. H. Rank, A. H. Guenther, G. D. Saksena, J. N. Shearer, and T. A. Wiggins, J. Opt. Soc. Am. 47, 686 (1957).

⁶E. K. Plyler, L. R. Blaine, and W. S. Conner, J. Opt. Soc. Am. 45, 102 (1955).

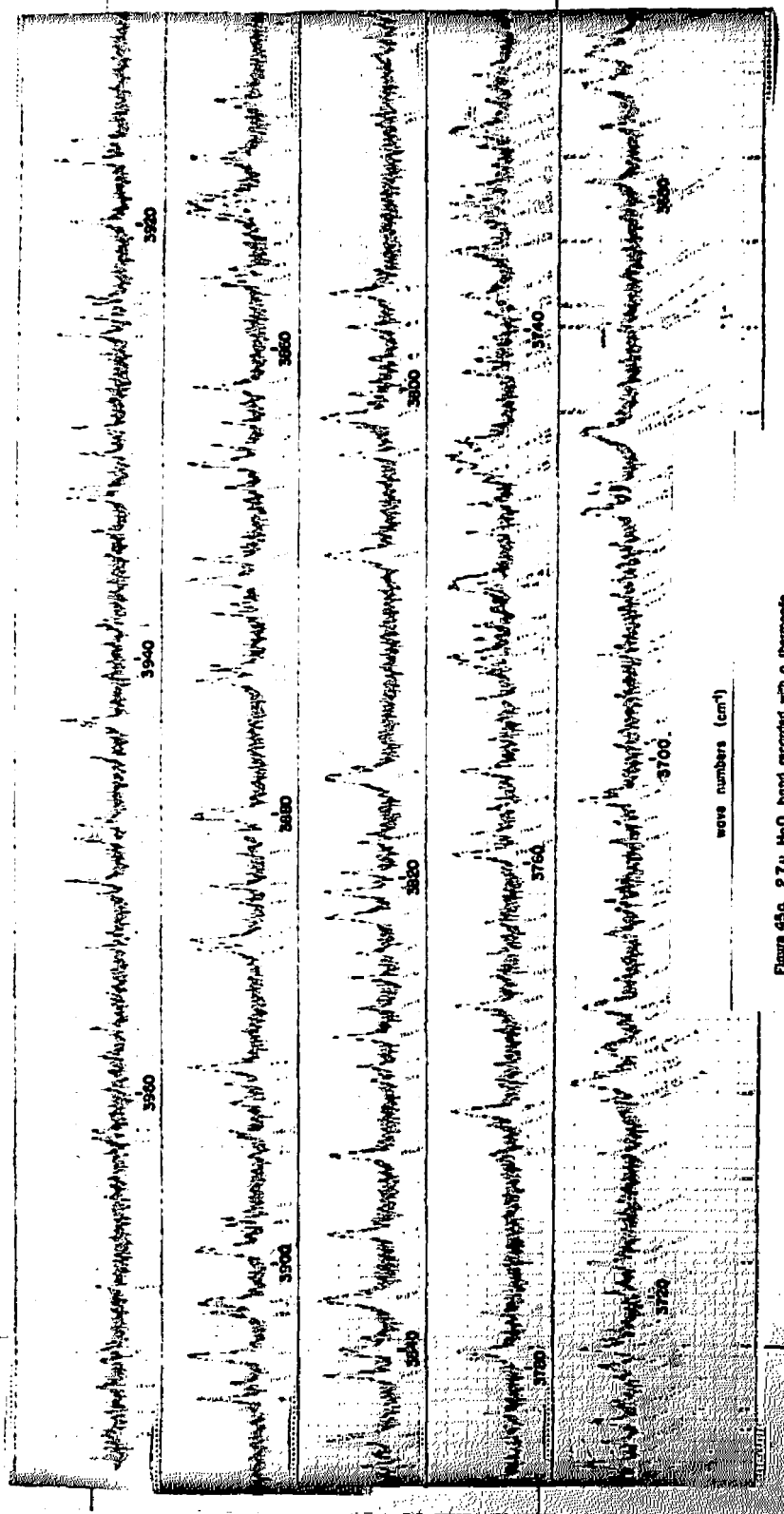


Figure 45a. 2.7 μ H₂O band recorded with a thermopile

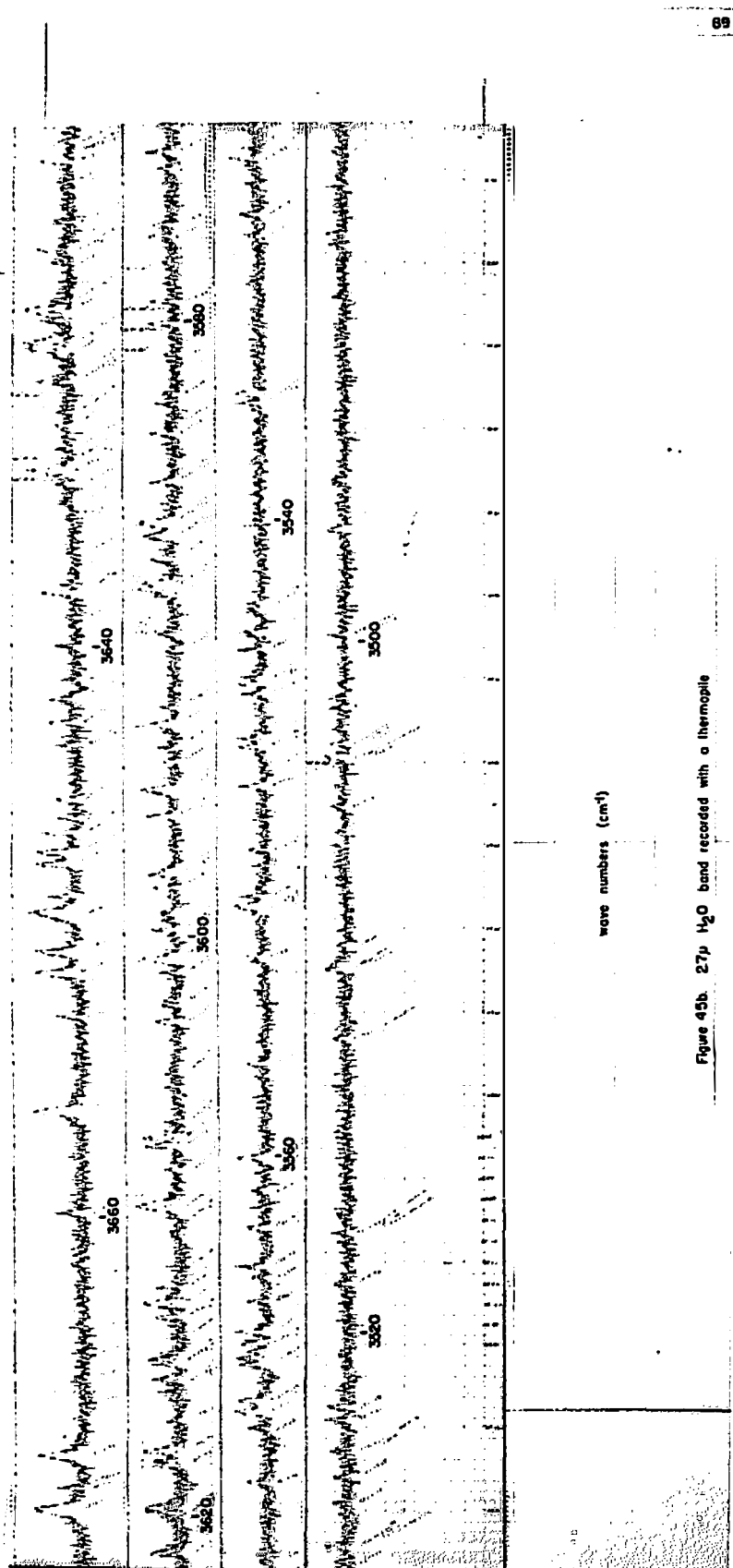


Figure 45b. 27μ H₂O band recorded with a thermopile

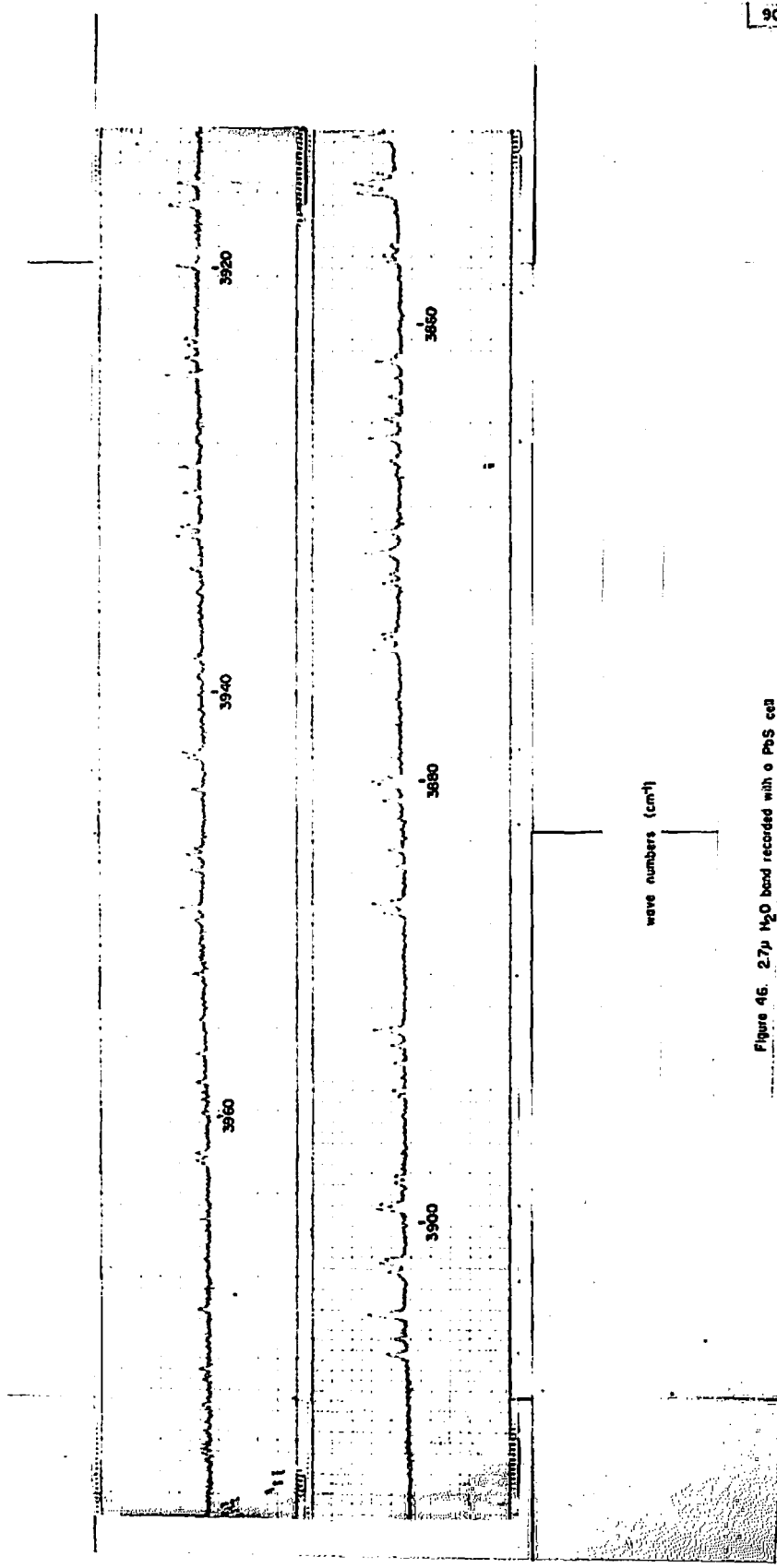


Figure 46. 2.7 μ H_2O band recorded with a PbS cell

records obtained of the 2.7μ band of H_2O . These records were obtained using a water vapor pressure of 2 to 3 mm. of Hg in an absorbing path of $8\frac{1}{2}$ meters. They were obtained with a 15,000 lines-per-inch grating using a grating speed of half a degree per hour and a spectral slit width of 0.085 cm^{-1} . The pressure in the instrument was first reduced to one-tenth of a millimeter of Hg, and then a small amount of water was admitted to the entire system until a pressure of 2 to 3 mm. of Hg was obtained. Figures 45 a and b show the region from 3980 cm^{-1} to 3500 cm^{-1} recorded using a thermopile as the detector, and Figure 46 shows the region from 3980 cm^{-1} to 3860 cm^{-1} recorded with a PbS cell as the detector.

Although only a small part of the band was observed with the PbS cell, it will be noted that the signal to noise ratio is considerably better with this detector than with the thermopile. This difference in the signal to noise ratios of the two detectors is an inherent characteristic and does not result from the quality of the optics. A clearer record would have been obtained of the entire region if it could have been recorded with the PbS cell, but unfortunately the sensitivity of the PbS cell falls off rapidly toward lower wave numbers and only a part of $2.7\mu\text{ H}_2\text{O}$ spectrum could be obtained. Only a small section of the PbS record is reproduced in Figure 46 for comparison.

Figure 47 is a photographic reproduction of this same absorption band recorded on the high-resolution vacuum-grating spectrograph of The Ohio State University using a PbS cell as the detector. These data obtained from the spectrograph at The Ohio State University are believed

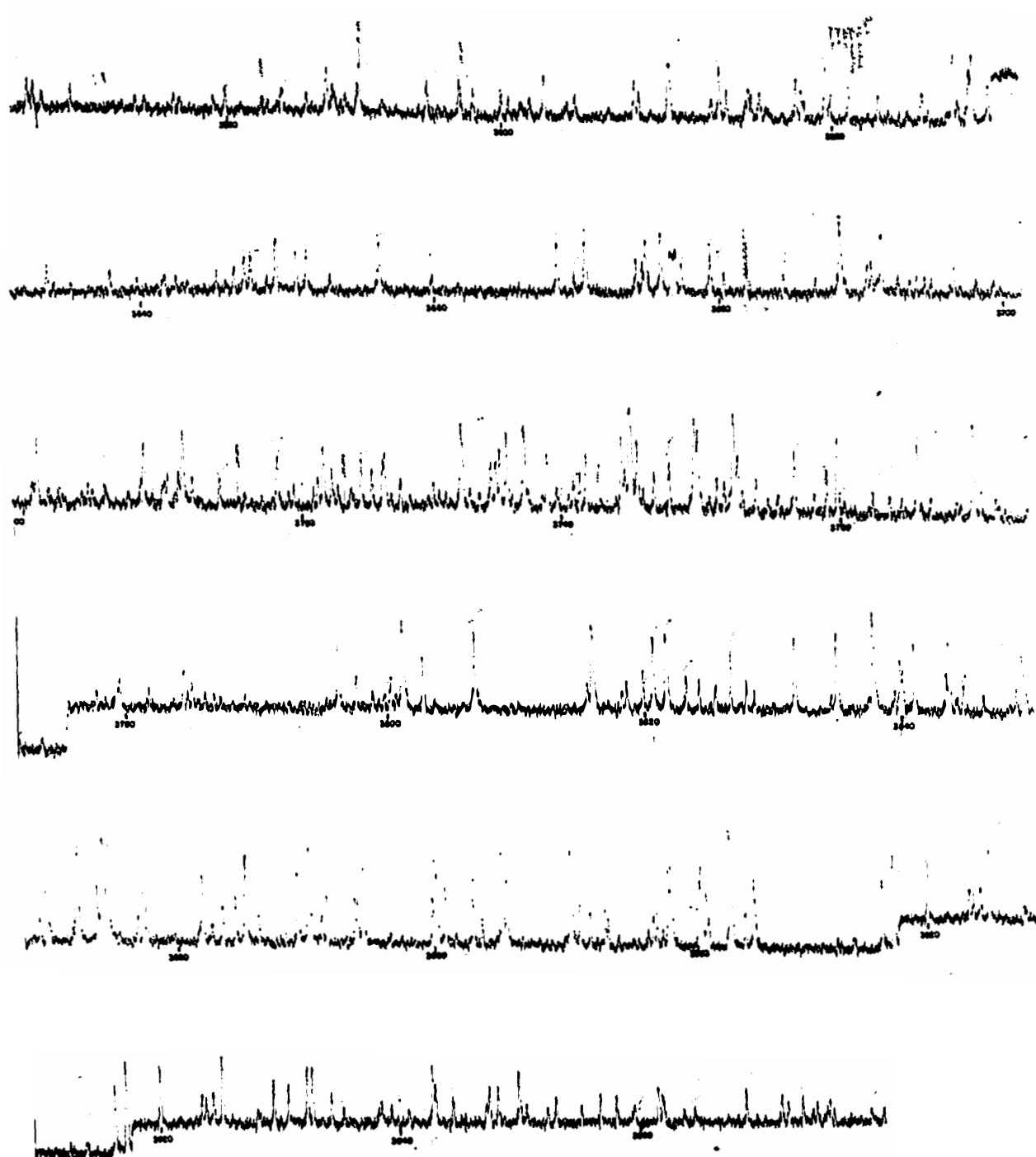


Figure 47. 2.7M H₂O recorded at The Ohio State University

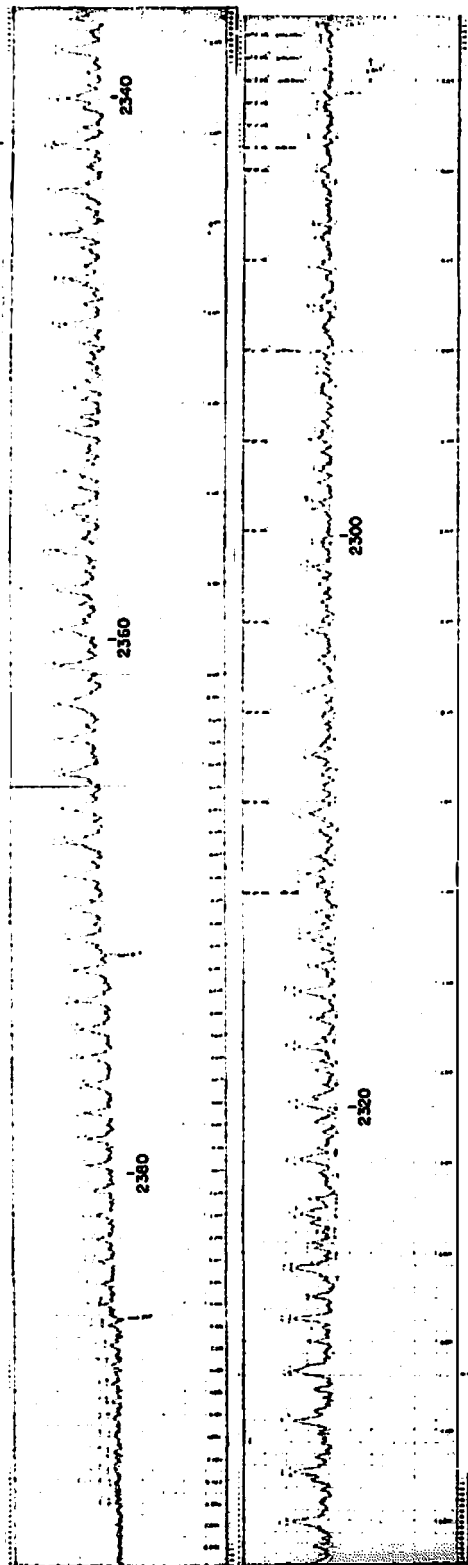
to be as good as any existing record on this particular band. A comparison of Figures 45 and 47 shows that the record made with the University of Tennessee's new spectrograph reproduces in every detail the record from the instrument at The Ohio State University. It will be observed in these records that lines with a separation of the order of 0.1 cm^{-1} are easily discernible. Two examples of this are observed at 3732 cm^{-1} and 3726 cm^{-1} . Lines with a closer spacing than 0.1 cm^{-1} are not resolved in these records, and it is believed that the low signal to noise ratio of the detectors is responsible. When more sensitive detectors become available and when the double pass instrument is completed, one would expect to be able to resolve lines with a spacing somewhat under 0.1 cm^{-1} .

The 4.25μ Carbon Dioxide Band

Figure 48 is a photographic reproduction of the record obtained on the 4.25μ band of CO_2 . This record was obtained using a carbon dioxide pressure of 1.0 mm. of Hg in an absorbing path of $8\frac{1}{2}$ meters. The record was obtained with a 7500 lines-per-inch grating using a grating speed of half a degree per hour and a spectral slit width of 0.1 cm^{-1} . A thermopile was used as the detector. The carbon dioxide pressure of 1.0 mm. of Hg was obtained by reducing the pressure in the instrument to one-tenth of a millimeter of Hg and then allowing a small amount of dry ice to sublime into the entire system.

Figure 49 is a reproduction of a record of the same region made by A. H. Nielsen and Y. T. Yao⁷ on a non-vacuum spectrometer

⁷A. H. Nielsen and Y. T. Yao, op. cit.



wave numbers (cm⁻¹)

Figure 48 ν_3 at 4.25μ for CO₂

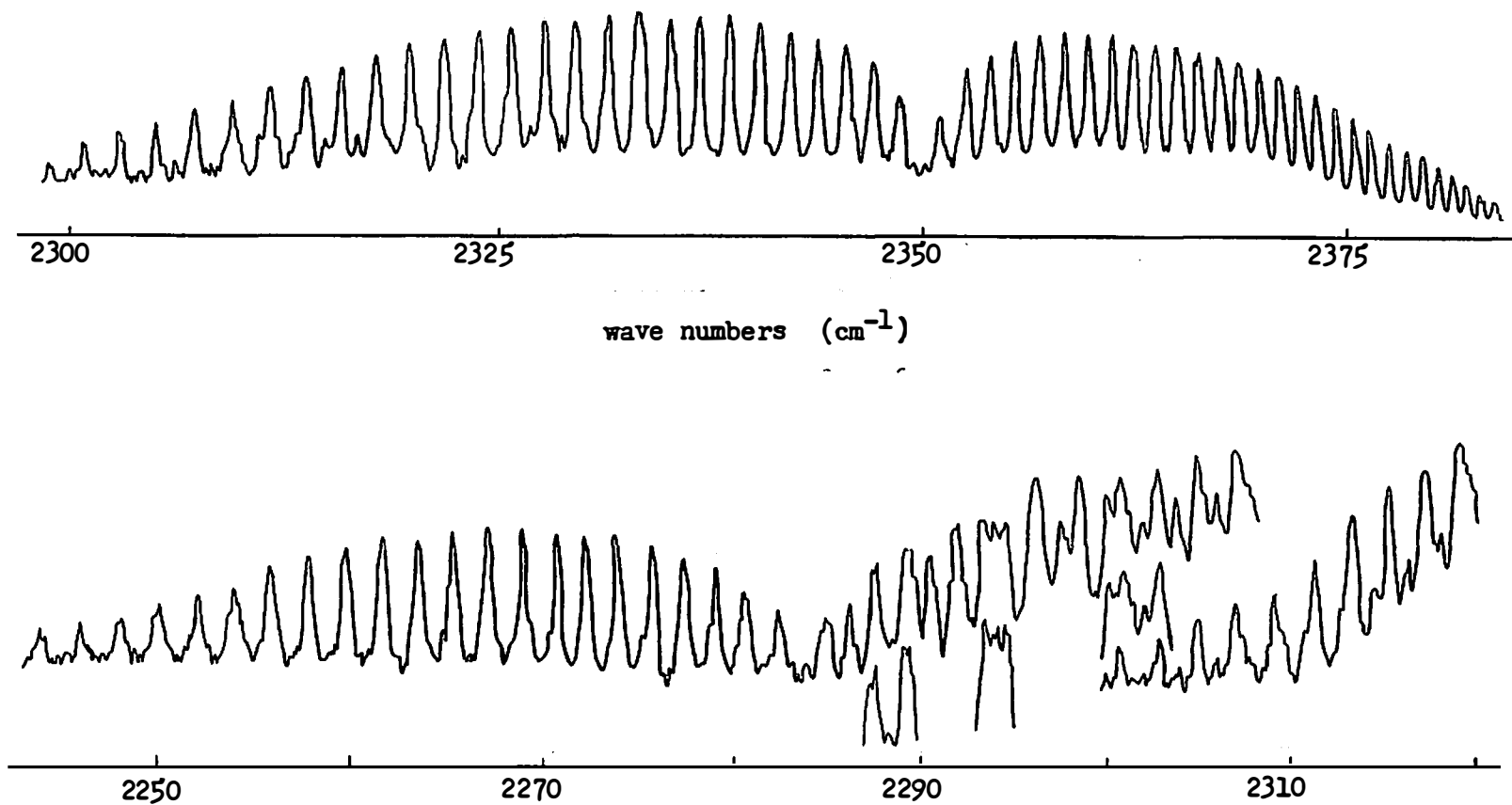


Figure 49. 4.25 μ band of CO₂ as recorded by Nielsen and Yao

which did not allow accurate control on the pressure of the absorber. This record was made before the days of automatic recording by taking many galvanometer deflection measurements at closely spaced intervals and then plotting the average deflections against wave numbers. The measurements were made by taking the average galvanometer deflection at a given grating position and then advancing the grating by five seconds of arc and taking the next reading. These readings were then plotted against wave numbers and a smooth line was drawn through them. It is evident that this type of measurement has inherently lower resolving capabilities than an automatic recording instrument because of the interval between measurements.

It will be noted in Figure 49 that the lines in the region from 2280 cm^{-1} to 2320 cm^{-1} are not clean. This results from the overlap of the $\text{C}^{13}\text{O}_2^{16}$ and $\text{C}^{12}\text{O}^{16}\text{O}^{18}$ isotopic bands of $\text{C}^{12}\text{O}_2^{16}$ and the possible presence of a "hot" band of $\text{C}^{12}\text{O}_2^{16}$ in this region. With accurate control of the pressure and higher resolution it is now possible to distinguish these bands thus allowing more accurate measurements to be made on the P lines of $\text{C}^{12}\text{O}_2^{16}$ out to $P = 68$, Figure 48. With this improvement in the values of the P lines it will now be possible to determine more accurately the molecular constants of the molecule, particularly the centrifugal stretching constant. It is also possible now to measure the lines of the isotopic bands and "hot" band and determine their band centers.

The 3.05μ Acetylene Band

Figure 50 is a photographic reproduction of the record obtained

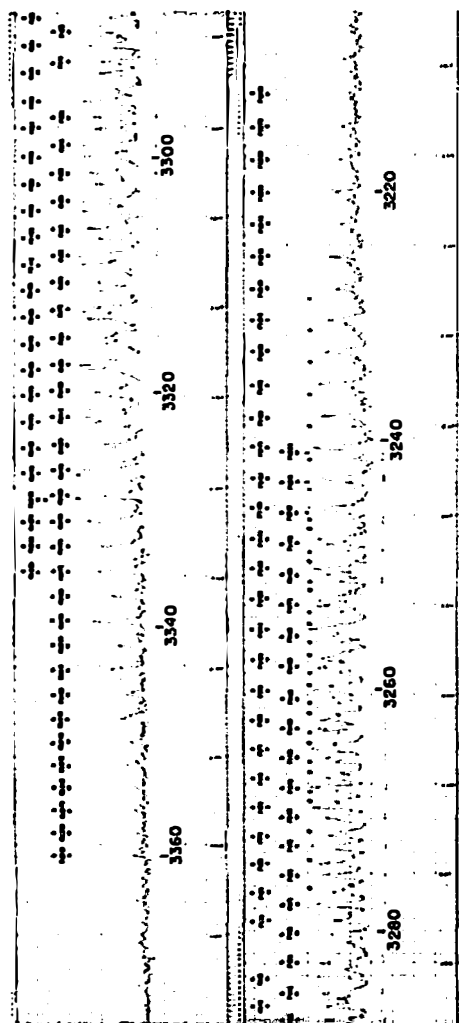
of the 3.05μ band of C_2H_2 . This record was obtained using a C_2H_2 pressure of 3 mm. of Hg in a 10 cm. absorption cell and a thermopile as the detector. The band was recorded with a 7500 lines-per-inch grating using a grating speed of one degree per hour and a spectral slit width of 0.15 cm^{-1} . The pressure in the instrument was reduced to about one-tenth of a millimeter of Hg to eliminate the absorptions of atmospheric H_2O which occur in this region.

Figure 51 is a reproduction of a record of the same region made by F. L. Keller⁸ on the University of Tennessee's non-vacuum prism-grating spectrograph. This record obviously was made with too much gas in the cell which accounts for some of the lack of resolution. Keller's measurements were made from slower speed records made with less gas.

It will be noted in Figure 51 that there are at least two absorption bands in this region, but they overlap in most of the region, and the resolution is not sufficient to allow accurate measurements to be made on most of the lines. Keller obtained sufficient data from his records to identify the ν_3 and $\nu_2 + \nu_4 + \nu_5$ absorption bands and to determine their band centers.

An examination of Figure 50 discloses that there are at least four different bands in this region, and perhaps a fifth. The lines of four bands have been distinguished and are lettered a, b, c, and d. The band centers of a and b have been determined and many of the

⁸F. L. Keller, op. cit., p. 77.



wave numbers (cm^{-1})

Figure 50 305 μ region of C_2H_2

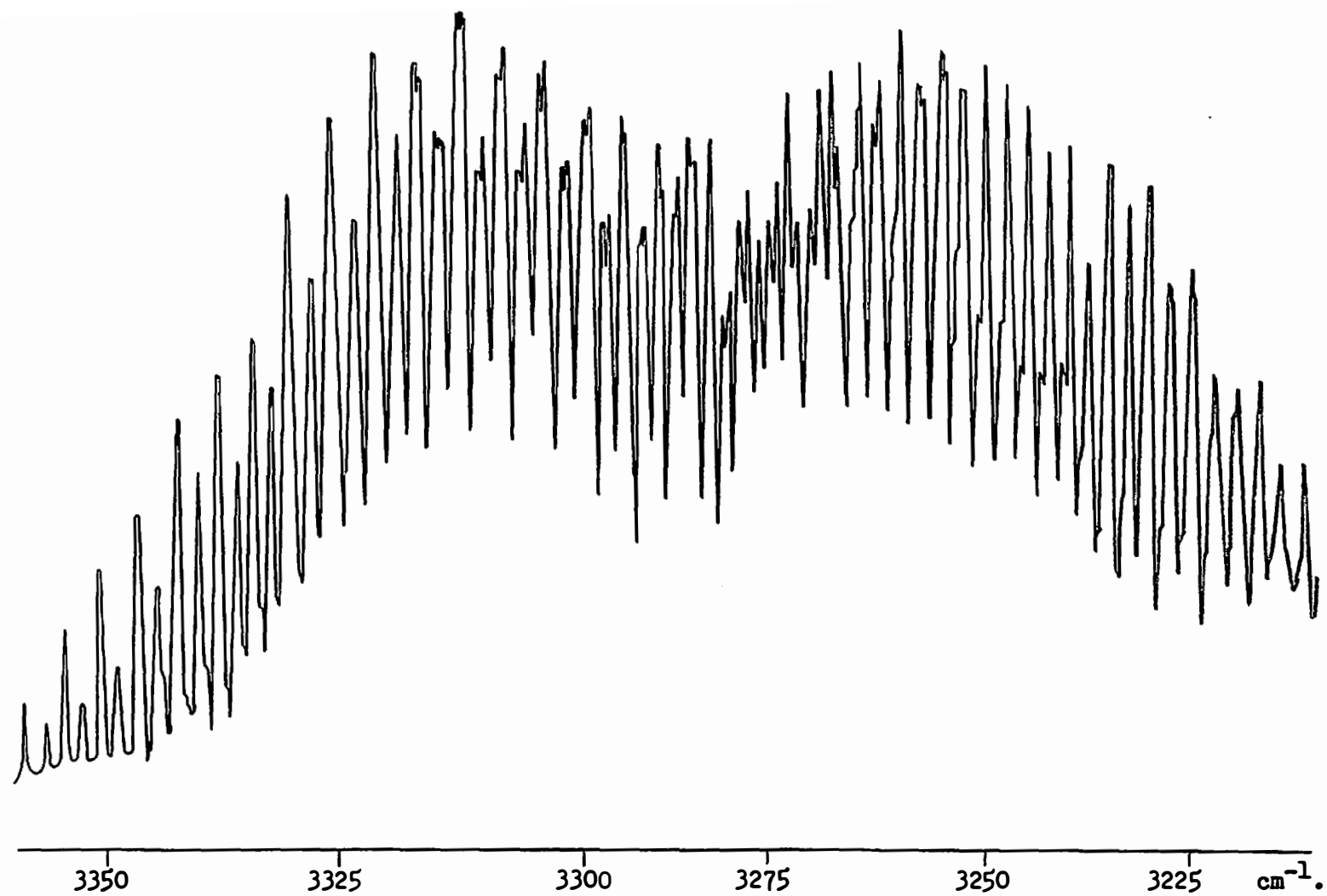


Figure 51. 3.05 μ region of C₂H₂ (after Keller)

rotational lines are identified. The band a is the ν_3 vibration-rotation band, and b is the $\nu_2 + \nu_4 + \nu_5$ band. These two bands were identified by Keller and, although he was not able to observe the weak R(0) line of the ν_3 band, it is clear from the new record that his interpretation of the band centers is correct. This weak R(0) line is clearly resolved in Figure 50. It will be noted that both the ν_3 and $\nu_2 + \nu_4 + \nu_5$ bands display an alternation in intensity in their rotational lines. This is characteristic of a $\sum_u^+ - \sum_g^+$ transition as discussed by Keller⁹. The energy level diagram for this type of transition is reproduced in Figure 52. In the ground state the even-numbered J levels have a lower statistical weight than the odd-numbered J levels, and in the upper state the odd-numbered J levels have a lower statistical weight than the even-numbered ones. The selection rule for transitions between the two levels is $\Delta J = \pm 1$, and the result is that the odd-numbered P and R lines are more intense than the even-numbered ones. This is indicated in Figure 50 by the letters s and w below the line designations.

The two bands lettered c and d do not seem to display an alternation in intensity, and it is possible that they are of the $\pi - \pi$ type; however, no Q branches appear obvious. These bands could also be "hot" bands, isotopic bands or weak combination bands. If they are "hot" bands they should weaken upon cooling of the sample and become enhanced on heating. If they do not weaken upon cooling and become enhanced on heating, then they are either weak combination bands

⁹F. L. Keller, op. cit. p. 32.

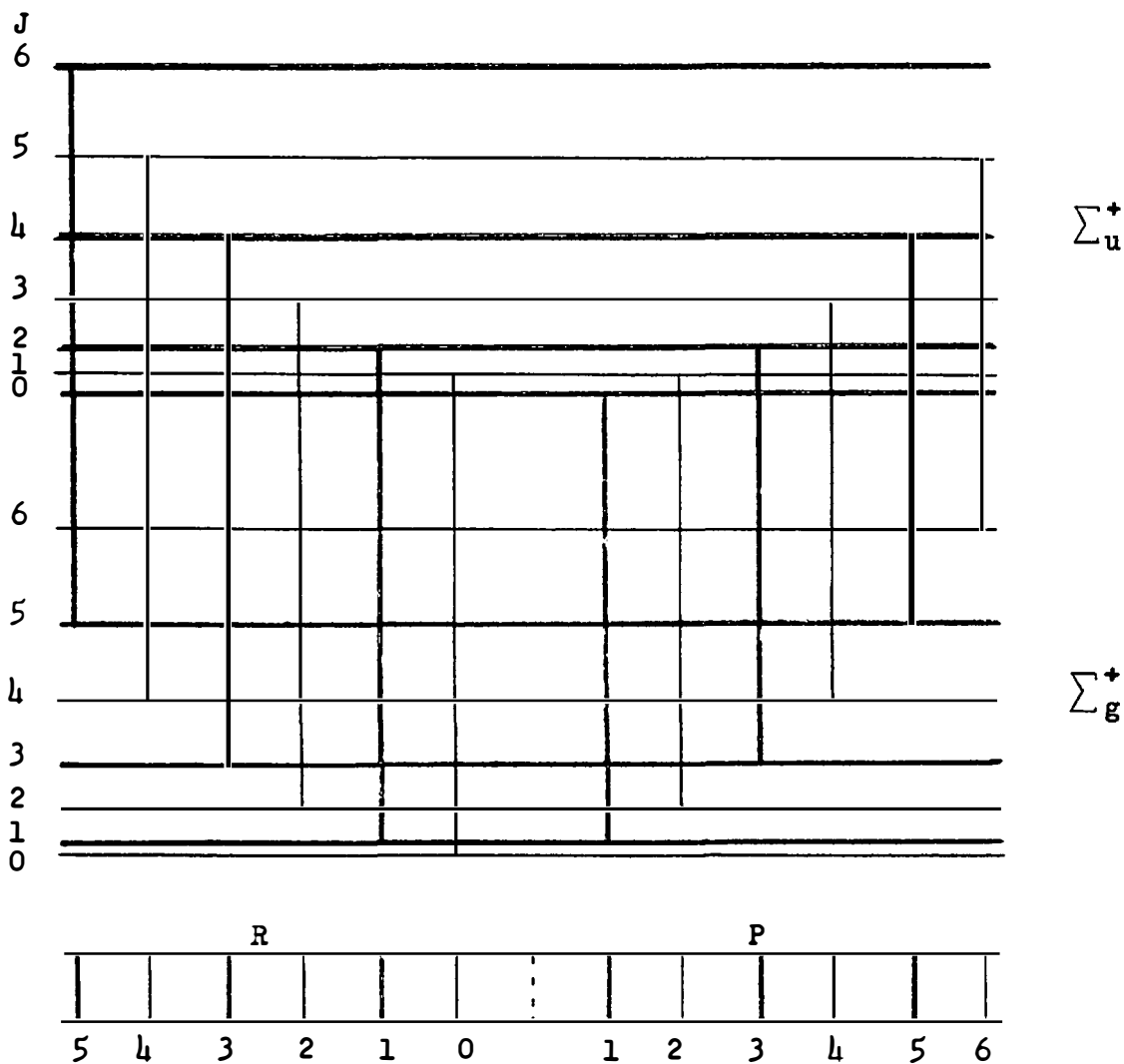


Figure 52. The $\Sigma_u^+ - \Sigma_g^+$ band

or isotopic bands. In any case it should now be possible to identify them by a more careful analysis of the spectrum. There are also numerous other regions in C_2H_2 which should be reexamined under these improved conditions.

It is clear from the comparison of these two records that the new instrument produces substantially better data than that obtained previously in this laboratory, and it will now be possible to obtain

better analyses and more accurate constants for many molecules.

The 2.35 μ Band of Carbon Monoxide

Figure 53 is a photographic reproduction of the record obtained of the 2.35 μ band of CO. This record was obtained using a CO pressure of one atmosphere in a 10 cm. absorption cell and using a PbS cell as the detector. The band was recorded along with the Fabry-Perot interference pattern and two standardized krypton lines¹⁰ using a 15000 lines-per-inch grating and a grating speed of one degree per hour. The spectral slit width was 0.2 cm⁻¹. The Fabry-Perot interference pattern was recorded using a C100 zirconium arc lamp as the source and a 1P22 multiplier phototube as the detector. The etalon plate spacing was about 2.5 mm., and it was used in fourth order, giving a fringe spacing of 0.5299 cm⁻¹. A No. 3-67 Corning filter was used to eliminate higher orders, and the pressure in the instrument was reduced to one-tenth of a millimeter so that vacuum wave numbers would be obtained.

The 13,151.599 cm⁻¹ and 12,322.65 cm⁻¹ krypton lines were used in third order for standards. The values of these lines were corrected for vacuum from the values of Plyler, Blaine, and Tidwell¹¹ by means of the Edlén dispersion formula¹².

¹⁰E. K. Plyler, L. R. Blaine, and E. D. Tidwell, J. Res. Nat. Bur. Stand. 55, 279 (1955).

¹¹Ibid.

¹²B. Edlén, J. Opt. Soc. Am. 43, 339 (1953).

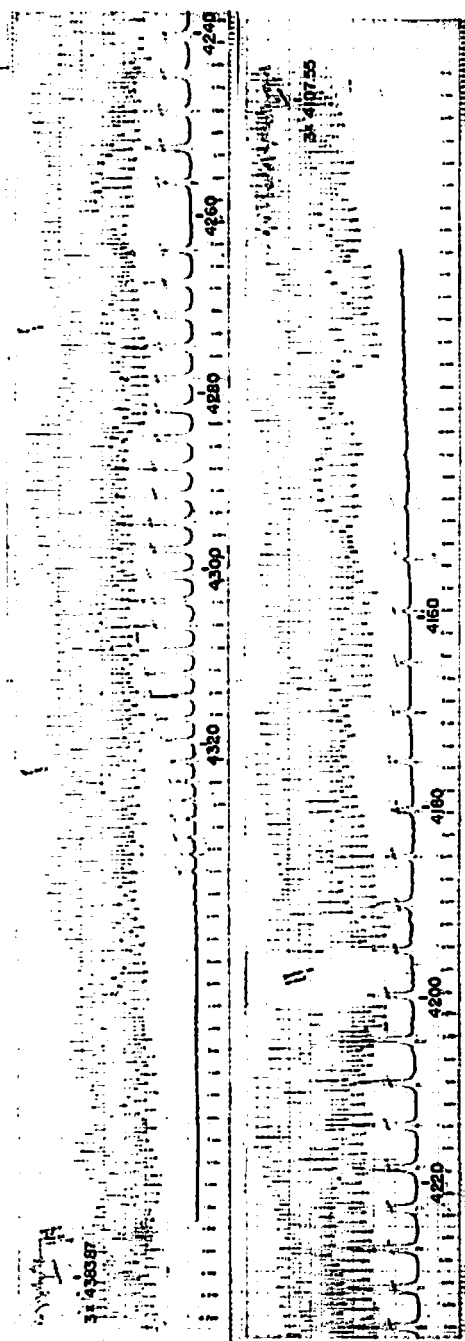


Figure 53. The 2.35 μ CO band

When measurements of the CO lines were made from this record using the two krypton lines as standards, the values obtained were shifted from the accepted values^{13, 14}. It will be noted that the krypton lines in Figure 53 are quite weak, and a close examination indicated that the $3 \times 4383.87 \text{ cm}^{-1}$ krypton line could not be marked accurately because of the high noise level. The CO lines were, therefore, remeasured using the R(0) line of CO, which is itself a secondary standard, and the $3 \times 4107.55 \text{ cm}^{-1}$ line of krypton. The average fringe spacing was calculated from these two lines and the other CO lines were assigned wave numbers relative to the R(0) line. The results of this measurement were much better than the results using the two krypton lines as standards. These results are given in Table IV.

The values in most cases agree within 0.04 cm^{-1} with the accepted values; however, a few of the lines deviate more than this. This lack of agreement is attributed to two factors. First, it is known that the temperature of the Fabry-Perot etalon was changing during the first part of the record causing the interference spacing to decrease slightly, and secondly a small portion of an interference ring was used rather than the central part of the interference pattern, and it is believed that the change in temperature caused the fringe system to shift slightly with respect to the entrance slit.

These difficulties can certainly be eliminated, and the statistics obtained from additional records should improve the accuracy to $\pm 0.01 \text{ cm}^{-1}$ or better.

¹³Rank, Guenther, Saksena, Shearer, and Wiggins, op. cit.

¹⁴Plyler, Blaine, and Comer, op. cit.

TABLE IV
MEASURED CO WAVE NUMBERS

Line	$\tilde{\nu}$ observed	$\tilde{\nu}$ standard	Δ^{**}	Line	$\tilde{\nu}$ observed	$\tilde{\nu}$ standard	Δ^{**}
R (0)	4263.84 [*]	4263.84	.00	P (1)	4256.20	4256.22	-.02
R (1)	4267.56	4267.54	.02	P (2)	4252.30	4252.30	.00
R (2)	4271.16	4271.18	-.02	P (3)	4248.36	4248.32	.04
R (3)	4274.74	4274.74	.00	P (4)	4244.31	4244.26	.05
R (4)	4278.24	4278.23	.01	P (5)	4240.22	4240.14	.08
R (5)	4281.67	4281.66	.01	P (6)	4236.02	4235.95	.07
R (6)	4285.00	4285.01	-.01	P (7)	4231.74	4231.68	.06
R (7)	4288.31	4288.29	.02	P (8)	4227.38	4227.35	.03
R (8)	4291.53	4291.50	.03	P (9)	4222.95	4222.95	.00
R (9)	4294.67	4294.63	.04	P (10)	4218.47	4218.48	-.01
R (10)	4297.70	4297.70	.00	P (11)	4213.94	4213.94	.00
R (11)	4300.69	4300.69	.00	P (12)	4209.36	4209.33	.03
R (12)	4303.63	4303.62	.01	P (13)	4204.68	4204.66	.02
R (13)	4306.47	4306.47	.00	P (14)	4199.92	4199.92	.00
R (14)	4309.27	4309.24	.03	P (15)	4195.20	4195.10	.10
R (15)	4311.94	4311.95	-.01	P (16)	4190.24	4190.23	.01
R (16)	4314.55	4314.59	-.04	P (17)	4185.31	4185.28	.03
R (17)	4317.11	4317.14	-.03	P (18)	4180.30	4180.26	.04
R (18)	4319.63	4319.63	.00	P (19)	4175.22	4175.18	.04
R (19)	4322.07	4322.05	.02	P (20)	4170.11	4170.03	.08
R (20)	4324.44	4324.39	.05	P (21)	4164.83	4164.81	.02
R (21)	4326.73	4326.66	.07	P (22)	4159.49	4159.53	-.04
R (22)	4328.94	4328.85	.09	P (23)	4154.20	4154.18	.02
R (23)	4331.06	4330.98	.08	P (24)	4148.70	4148.76	-.06
R (24)	4333.05	4333.03	.02				
R (25)	4335.02	4335.00	.02				

^{*}The other lines are measured relative to this line.

^{**} $\Delta = \tilde{\nu}$ observed - $\tilde{\nu}$ standard.

CHAPTER V

DIFFICULTIES AND SUGGESTED IMPROVEMENTS

In the process of testing the instrument a number of difficulties were encountered. The following sections describe these difficulties, indicate what has been done to correct them, and give suggestions for further improvement.

Amplifier Noise

When the instrument was completed the infrared detecting and recording system was tested with the instrument at atmospheric pressure. The system was run for a number of hours to be certain that all of the components were operating satisfactorily. The instrument was then evacuated, and the testing was continued. After about four hours the system suddenly became very noisy, and it was observed that this noise could be temporarily eliminated by switching the chopper off and on. The vacuum system was then opened, but the noisy condition continued. The chopper rectifier contacts were then cleaned with alcohol, and the noise level dropped to normal and remained there as long as the system was operated at atmospheric pressure. Subsequent tests revealed that the noise level would remain normal as long as the system was operated at atmospheric pressure and that it would return in two to six hours after the system was evacuated.

It was postulated that the breaker points arced slightly in vacuum and slowly built up an insulating coating on the contacts. To

reduce the arcing 0.05 mfd. capacitors were put across the breaker contacts and the testing was continued. Since the installation of the capacitors the instrument has been operated under vacuum for about twenty hours, and the noisy condition has not returned.

It is recommended that the breaker contacts of both the infrared and Fabry-Perot systems be cleaned periodically to keep the noise level at a minimum and prevent the noisy condition from occurring.

Zirconium Arc Source

The original zirconium arc source was housed in a glass cooling jacket and had a sapphire window so that it could be used as an infrared source. Unfortunately this source burned out in less than three hours of operation, and it had to be replaced with a regular C100 zirconium arc lamp. A special metal cooling jacket was built to house these lamps and prevent the unwanted radiation from heating up the system. The life of these lamps is greatly reduced by operation in vacuum because there is no convection cooling. Their average life in vacuum is about ten hours.

It has been suggested that the life of these lamps might be increased by applying a black coating to the inside of the cooling jacket to reduce the amount of radiation reflected back onto the lamp. This has not yet been done but undoubtedly will be tried in the near future.

Standard Emission Lines

It has been observed that the emission lines from the krypton arc are often too weak to be observed when there is an absorption cell in the light path. This undoubtedly results from scattering of the visible krypton light by the cell windows. This condition could be greatly improved if a device were provided for removing the absorption cell from the light path while the standard emission lines are being recorded. Another possibility, of course, would be to obtain more intense arc sources, but this may present the problem of cooling the source to prevent the envelope from melting. In any case more work needs to be done on this problem of obtaining more intense standard emission lines.

The Mirror Rotating System

The mirror rotating system described in Chapter III has been found to be much too sensitive, making it difficult to get the light to fall on the entrance slit to the prism monochromator. This has been improved by putting stops on the rotating shaft, however, it is still not entirely satisfactory.

Two possible solutions to this problem are 1) to increase the gear ratio between the synchro repeater and the rotating mirror shaft by using a worm and worm gear in place of the spur gears, and 2) to eliminate the rotating mirror entirely and mount the sources on a rotating table. If the sources were mounted on a rotating table more than two sources could be brought into play without opening the

vacuum, and the same external control system could be used to select the desired source.

Temperature Variation of the Fabry-Perot Etalon

In checking the performance of the Fabry-Perot system it was observed that the fringe spacing decreased slowly over a long period of time while the instrument was in operation. This effect was traced to the chopper motors which were found to become quite warm when running in vacuum. The heat was slowly transmitted to the etalon causing the plate spacing to increase resulting in a decrease in the fringe spacing. To reduce this heating effect, insulating spacers were placed between the motors and their mounting frames, and cooling pads were fastened to the motors to conduct the heat away. This greatly reduced the amount of temperature variation at the etalon but did not eliminate it completely. The temperature of the etalon would reach equilibrium, however, after being operated for several hours in vacuum.

The temperature variation which is now present in the system is believed to be partially caused by radiation heating from both the zirconium lamp and the Nernst glower. This radiation heating would be difficult if not impossible to prevent.

It is suggested that the effect of the temperature variation could be reduced by making the etalon mount out of invar instead of stainless steel or by controlling the temperature of the present mount by means of a small heating coil and thermostat. It may turn out to be necessary to do both of these.

CHAPTER VI

CONCLUSIONS

It has been demonstrated that the new instrument will produce data which are substantially better than any previously obtained in this laboratory, and as good as that produced by comparable instruments in other laboratories. There are, however, a number of changes which should and undoubtedly will be made to improve its operation and performance.

The instrument is well built and is versatile enough to accept any improvements in detection and other techniques which may be developed in the future. It is believed that this spectrograph is as good as any comparable instrument in existence today.

BIBLIOGRAPHY

APPENDICES

APPENDIX A

INSTRUCTIONS FOR EVACUATING THE SPECTROGRAPH

Figure 54 is a diagram of the VSD-8-8-11 Kinney vacuum pump used in evacuating the spectrograph.

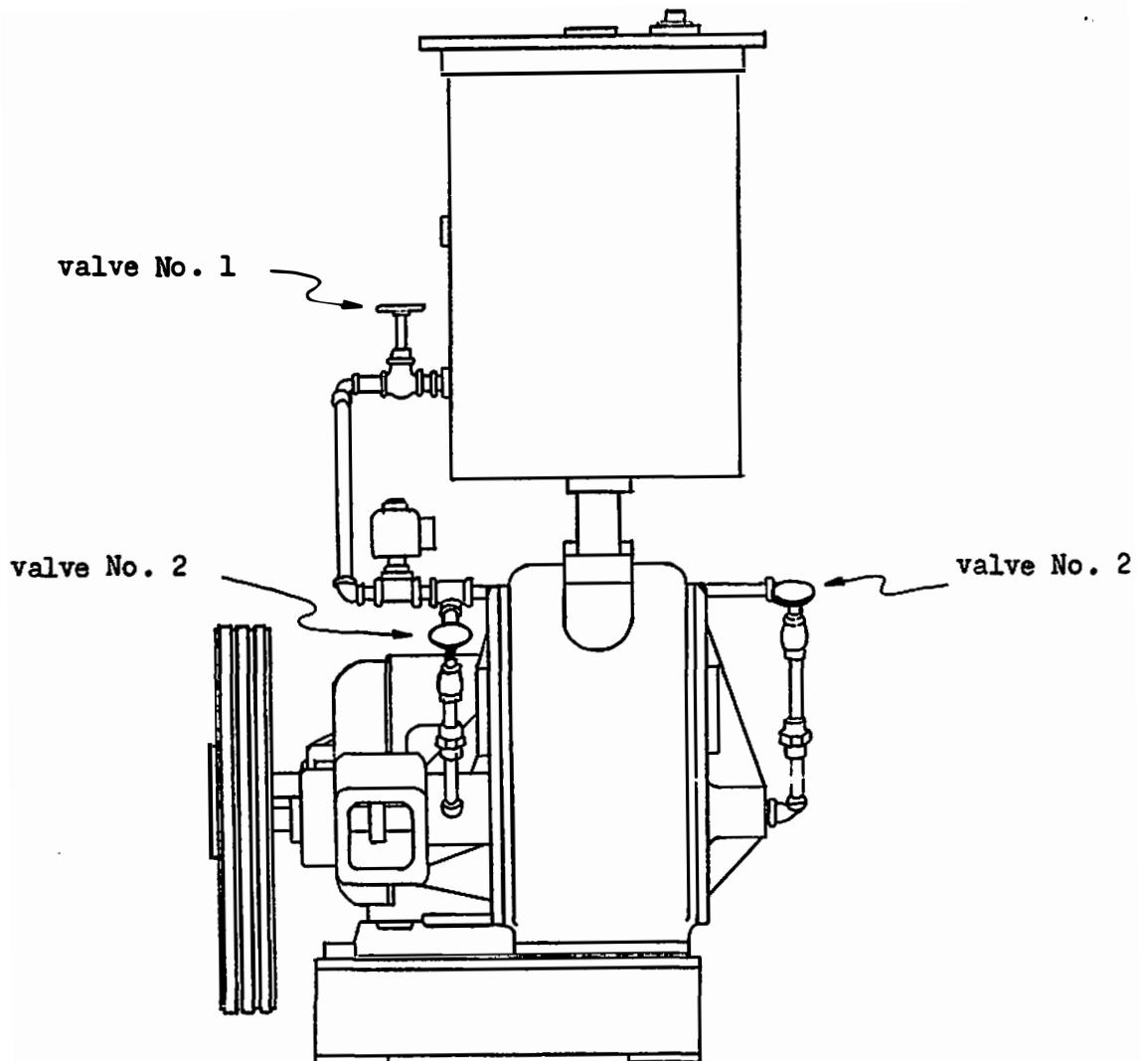


Figure 54. Kinney vacuum pump

Before starting the pump, bolt the tank closed to seal the gasket and check the air inlet valve at the head of the tank and the two inch vacuum valve to see that they are closed. Turn the pump over by hand to expel the oil from the pump chamber. See that valve No. 1 in the oil seal pipe is closed and remains closed until the pump is running under power, then open it wide. Check to see that valves No. 2 are opened from one to one and a half turns, then open the two inch vacuum valve in the pump line. When the pressure in the tank is reduced by about twenty centimeters of Hg the bolts will become loose and may be removed.

After the desired pressure is reached, close the two inch vacuum valve and valve No. 1. Allow the pump to run for about half a minute to clear itself of oil and then turn off the power.

The pressure in the tank is raised to atmospheric by opening the one inch vacuum valve at the head of the tank. The tank may then be opened in about ten minutes.

If the pressure cannot be reduced below 100 microns the vacuum oil may contain an excessive amount of water. This may be removed by operating the pump and bleeding a small amount of air through it by opening the needle valve in the side of the pump housing. It will usually take from four to eight hours to completely dry the oil.

APPENDIX B

GRATING DATA

At present four gratings are available for use in the spectrograph. The data for these gratings are given in Table V.

TABLE V

GRATING DATA

Lines/cm	Lines/inch	Blaze Angle	Approximate Grating Constant K_g
472.440	1200	24°	236.24 cm ⁻¹
1800.00	4572	23.5°	900.09
3000.00	7620	25.4°	1500.15
6000.00	15240	36.5°	3000.29

APPENDIX C

LUBRICATION IN VACUUM

The normal petroleum lubricants cannot be used in vacuum because they have a high vapor pressure and are soon carried out of the system by the vacuum pump, leaving the surfaces dry. It was, therefore, necessary to find a satisfactory lubricant having a low vapor pressure. A number of lubricants were tried, and some of these were found to be completely unsatisfactory. The lubricant which was finally chosen was a mixture of 25 per cent of Series 11-14 Halocarbon oil and 75 per cent of No. 14 fluid silicone grease. This lubricant has been used on all the moving parts in the system. It has been in the instrument almost a year now and has proved to be perfectly satisfactory.

APPENDIX D

INSTRUCTIONS FOR SETTING THE PRISM MONOCHROMATOR

The prism monochromator is provided with a rock salt prism and a linear wave number cam which is linear from 4000 to 700 cm^{-1} . At the 4000 cm^{-1} end of the cam there is a sharp dip which extends the range of the monochromator up into the visible region of the spectrum in a non-linear manner. The bottom of this dip has been chosen as the zero setting for the monochromator duodial. Figure 55 is a graph of the duodial settings for the wave number region from 4000 to 700 cm^{-1} . In this region the dispersion of the rock salt prism is sufficient to separate the various orders so that only one order is seen by the grating.

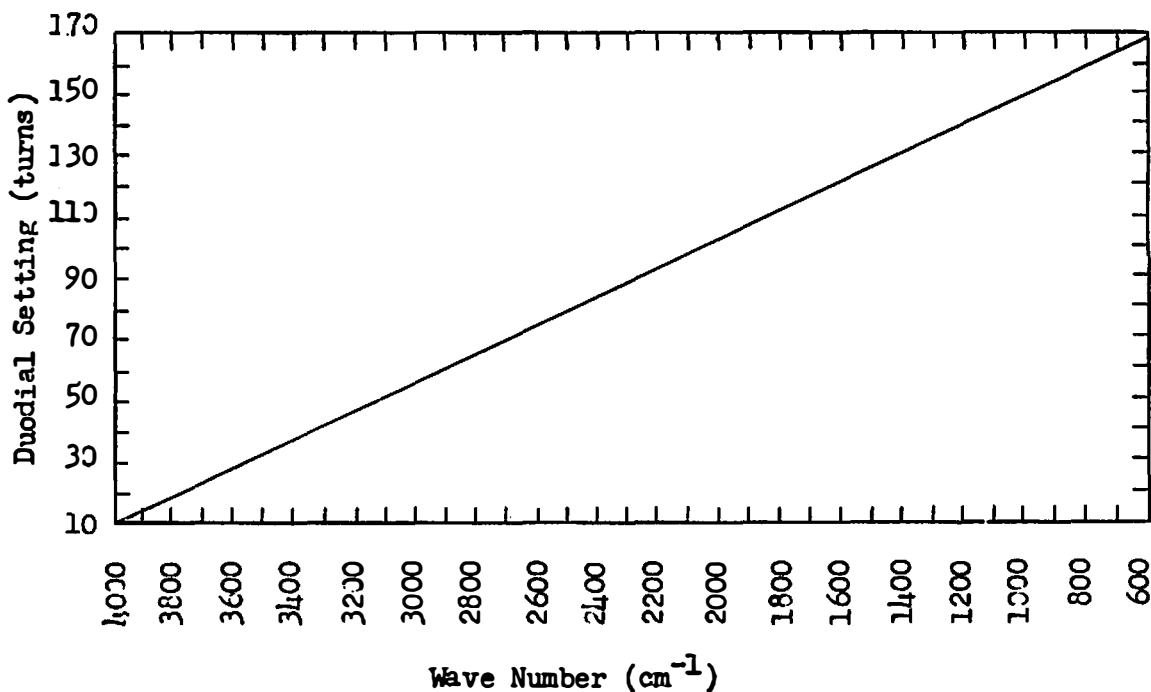


Figure 55. Prism monochromator settings

APPENDIX E

FILTER DATA AND DETAILS FOR OPERATING THE FABRY-PEROT SYSTEM

In operating the Fabry-Perot system a number of conditions must be satisfied if optimum performance is to be obtained. The alignment of the optical system is quite critical, and the following adjustments should be made with considerable care:

- 1) The Fabry-Perot etalon should be illuminated with parallel light. This adjustment can be made quite easily because of the high reflectivity of the Fabry-Perot plates. The light from the source passes through the collimating lens and is reflected by the first Fabry-Perot plate. The light returning through the lens is then focused at some point near the source. Parallel light is obtained by moving the collimating lens until this image coincides with the source.
- 2) The interference pattern of the Fabry-Perot must be in sharp focus on the entrance slit of the grating monochromator. This is accomplished by placing a plane mirror in front of the zirconium arc at 45 degrees to the optical axis and illuminating the etalon with sodium light. The adjusting screws on the Fabry-Perot plates are then turned until a sharp image of the pattern is obtained on a white card placed in front of the entrance slit. The central spot of the interference pattern will normally be used and the Fabry-Perot optical system should

be moved until this spot falls on the entrance slit. The sodium light is then replaced by the zirconium arc which is moved from side to side until the source is focused at the spot where the center of the pattern had been observed.

3) Once the infrared region of interest has been determined it is necessary to find out which order of visible light will give the best interferometer pattern. This is done by considering the range of the source and detector and the cut-off points of the available filters. Figure 56 is a graph for the 15000 lines-per-inch grating indicating the limits of the zirconium arc source and the 1P22 multiplier phototube together with the cut-offs of a number of filters. The graph is a plot of wavelength in microns versus the sin of the grating angle θ for the various orders of the grating. For example if the infrared region of interest lies at $\sin \theta = 0.7$ then one would use the visible light in fourth order. The cut-off of the 1P22 multiplier phototube would provide the upper cut-off to eliminate lower orders and a Corning No. 3-67 filter would be used to eliminate higher orders.

4) It is now necessary to determine the maximum slit setting for which the interferometer pattern will be detected. If the plate spacing is 0.25 cm., the fringe spacing in the infrared will be given by $\frac{1}{2nd}$ where n is the order of visible light used and d is the plate spacing. For $n = 4$ and $d = 0.25$ cm the fringe spacing $\Delta \lambda$ will be 0.5 cm^{-1} . The spectral slit width must now be set at less than 0.5 cm^{-1} if an interference pattern

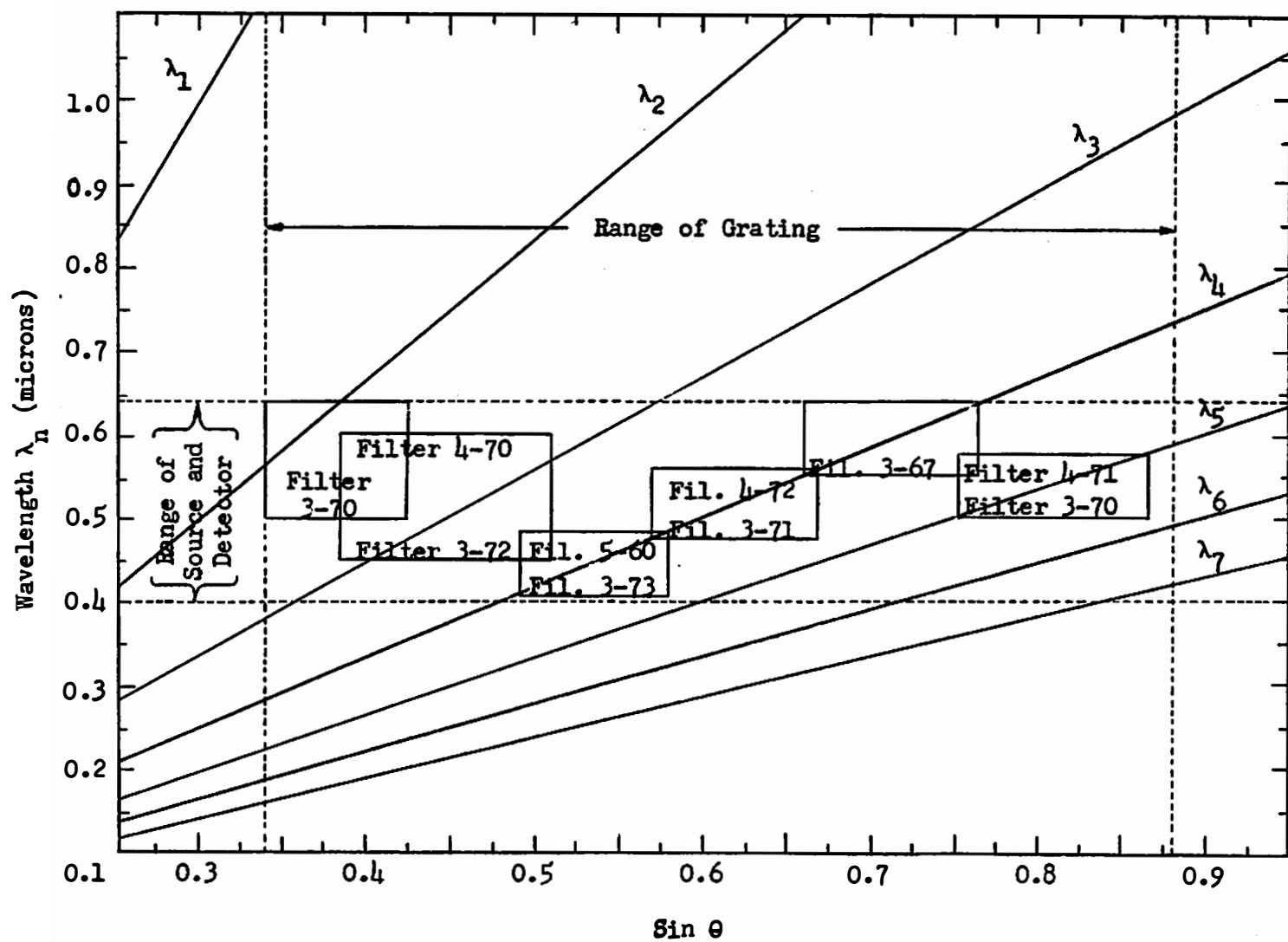


Figure 56. Filter data for the 15000 lines-per-inch grating

is to be detected. The spectral slit width s in millimeters is given by

$$s = \frac{2f\Delta\tilde{\nu}}{\tilde{\nu}} \tan \theta$$

where f is the focal length of the collimating mirror in the grating monochromator in millimeters, $\tilde{\nu}$ is the infrared wave number for which the grating is set, and θ is the grating angle.

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