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Calculated Spectra Resolution of Perkin-Elmer Prism and Grating Monochromators

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CONTENTS

ABSTRACT

A simple derivation of the spectral resolution of the standard Perkin-Elmer prism and grating monochromators (Models 12-C and 12-G) has been carried out. Some attention is given to discussion of the variation of the diffraction pattern width at the exit slit as a function of the physical width of the entrance slit. Brief mention of power considerations is also made. The resulting formulas have been used to calculate spectral slit width curves for eight different prisms and twenty-six gratings. The spectral slit width in cm^{-1} is plotted as a function of the frequency in cm^{-1} and wavelength in microns. These detailed graphs allow a determination of spectral slit width from quick inspection.

PROBLEM STATUS

This is an interim report on a continuing problem.

AUTHORIZATION

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CALCULATED SPECTRAL RESOLUTION OF PERKIN-ELMER PRISM AND GRATING MONOCHROMATORS

INTRODUCTION

In spectroscopic research problems a knowledge of the spectral slit widths used, i.e., that portion of the continuous spectrum thrown across the exit slit focal plane which gets through to the detector, is often necessary. The equations are developed here taking into account both the effects of finite slit width and diffraction of a limiting aperture. Extensive calculations for Perkin-Elmer monochromators such as Models 12-C and 12-G equipped with various prisms and gratings have been made. The results are presented graphically for convenient use in the laboratory. A brief mention of power received at the detector, in terms of various spectral parameters, is presented.

In Table 1 at the end of the text are listed the prisms for which calculations were made. The dimensions of the prisms are primarily those given in various Perkin-Elmer manuals. The indexes of refraction for these materials were obtained from a report by Ballard, McCarthy, and Wolfe (1). In Table 2 are listed the echelette gratings for which calculations were made. The gratings were obtained from Bausch and Lomb Optical Co., University of Michigan, and Farrand Optical Co. Much of the development is based on papers and books by the following authors: Brügel (2), Jenkins and White (3), Conn and Avery (4), Barnes, McDonald, Williams, and Kinnaird (5), Cross and Nixon (6), Schuster (7), and Von Keussler (8).

DEFINITION OF SPECTRAL SLIT WIDTH

To facilitate a simple discussion of spectral slit width, a schematic diagram of the prism monochromator optics is shown in Fig. 1. A grating monochrometer would be similar; if the prism is removed, we may consider the Littrow mirror in the grating position after slight modification of the collimating mirror. Ignoring diffraction effects and considering monochromatic radiation of wavelength λ_1, a geometrical image of the entrance slit is formed on the exit slit focal plane. Consider that the dispersion element (prism or grating) is adjusted to move this monochromatic image across the exit slit. For entrance and exit slits of equal widths, the signal observed by the detector is triangular in shape as a function of the motion of the dispersion element (angle of grating or prism) as illustrated in Fig. 2(a). This triangle is called the slit function. If another monochromatic wavelength λ_2 also illuminates the entrance slit, the detector signal is triangular also, as shown in Fig. 2(a). The two wavelengths λ_1 and λ_2 are separated physically in space because of the dispersion. All the energy detected under each triangle is of wavelength λ_1 or λ_2, respectively. We may now replace the horizontal scale with a wavelength scale as in Fig. 2(b). The two triangles are on the verge of resolution when the peak of one is over the edge of the other as shown in Fig. 2(c). In the overlap region the energy is a mixture of λ_1 and λ_2. The physical slit width expressed in terms of the wavelength (by calculation of the dispersion) may now be called the spectral slit width $\Delta\lambda$. In practice, the concept is more complicated since the image of the entrance slit is a diffraction pattern and the specific criterion for resolution is important. Also a distortion of the triangle is produced whenever the dispersion is not constant. A more thorough discussion of spectral slit width is given by Streiff and Ferriso (9).

Note: James R. Stevenson's permanent address is Georgia Institute of Technology, Atlanta, Georgia.

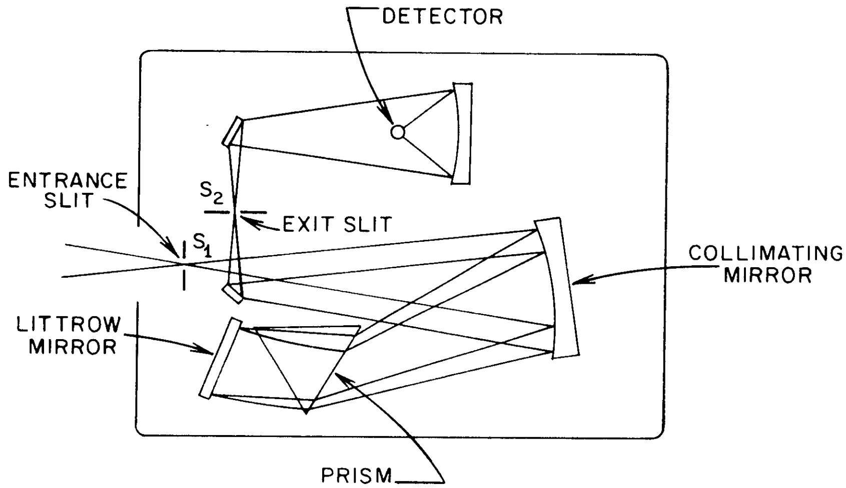

Fig. 1 - Schematic optical ray diagram of the prism monochromator

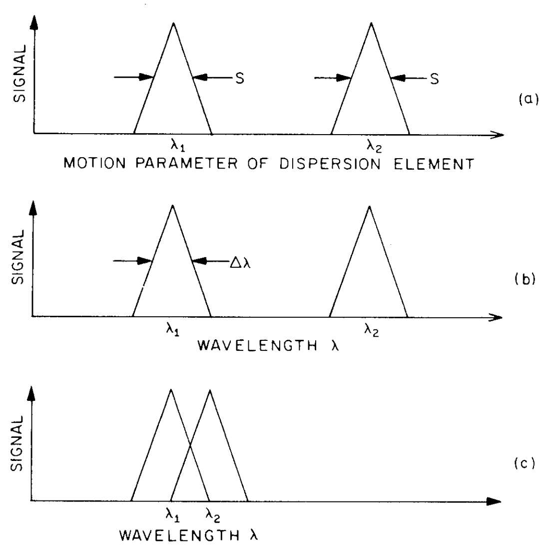

Fig. 2 - Triangular slit function used in the discussion of the spectral slit width

PRISM CALCULATIONS

The calculation of the spectral resolution or spectral slit width in the prism instrument is made under the assumptions that the Littrow mounting is used in which the light passes through the prism twice and that the prism is nonabsorbing. The prism is used close to the angle of minimum deviation. Optical abberations, prism absorption, and coherence effects are neglected. Figure 3 shows a schematic ray diagram in which S is the width of the entrance and the exit slit, f is the focal length of the collimator mirror or lens, D is the width of the collimated beam, b is the width of the prism base, A is the apex angle of the prism, and i is the angle of incidence. A collimating lens is used for simplicity. We neglect the angular separation δ of the two slits in subsequent calculations. Following Conn and Avery (4) we introduce a variable α defined as

$$\alpha = \frac{S/f}{\lambda/D}. \tag{1}$$

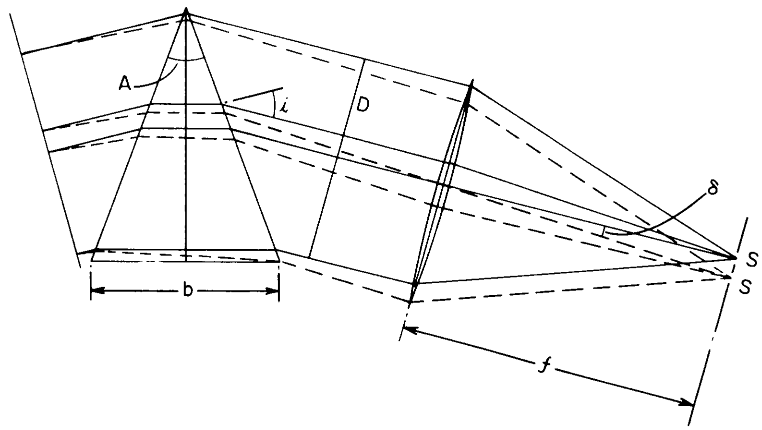

Fig. 3 - Schematic ray diagram for the Littrow mount

This variable differs by a factor of two from that defined by Conn and Avery. The numerator S/f is the angle subtended by the entrance or exit slit of width S on the collimating mirror of focal length f. The denominator λ/D is the angular half-width of the first diffraction maximum formed at the exit slit of an infinitesimal entrance slit, because the optical beam is limited to a width D by either the collimating mirror or the prism. These conditions result in Fraunhofer diffraction.

Fresnel diffraction of the converging beam at an entrance slit of finite width and depth is important when the wavelength becomes comparable to or larger than the slit width. In this case energy is lost from a beam of fixed solid angle, and there may be an effect on the resolution. This problem has been considered by Moore (10), and also by Bell, Burnside, and Dickey (11) in connection with power measurements with a Perkin-Elmer spectrometer, and is mentioned by Sawyer (12) in connection with the work of Van Cittert (13). Jones and Richards (14) have studied diffraction and polarization effects of slits. These papers refer to several of the more basic theoretical works pertaining to diffraction by apertures, especially when the aperture size is comparable to the wavelength.

In the present work we avoid the question of whether it is actually possible to produce a diffraction pattern of a point or line source that has a physical size less than the wavelength of the radiation being used.

We now simplify further by using the schematic ray diagram in Fig. 4a. The angular width $\Delta\theta$ of the monochromatic image of a finite entrance slit on the exit slit focal plane can be written as the sum of the geometric angular width $\Delta\theta_S$ and the extension due to diffraction $\Delta\theta_D$:

$$\Delta\theta = \Delta\theta_S + \Delta\theta_D . \tag{2}$$

Then from the definition of $\Delta\theta_S$ and α

$$\Delta\theta = \frac{S}{f} + \Delta\theta_D = \frac{\lambda\alpha}{D} + \Delta\theta_D . \tag{3}$$

This is illustrated schematically in Fig. 4b where an intensity pattern is shown for a geometrical image and the extended pattern due to diffraction. For optimum resolution, the exit slit should be slightly wider than the entrance slit. The extension of the image due to

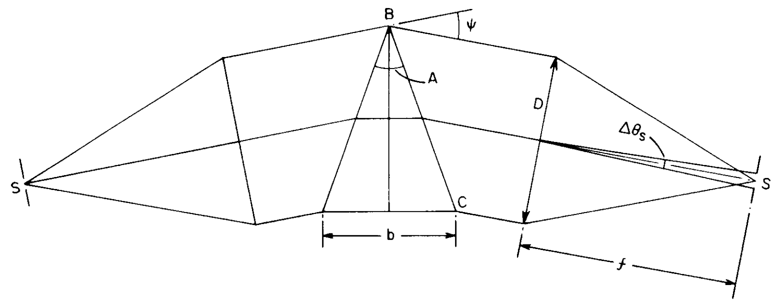

Fig. 4a - Simplified schematic ray diagram of the beam passing the prism once

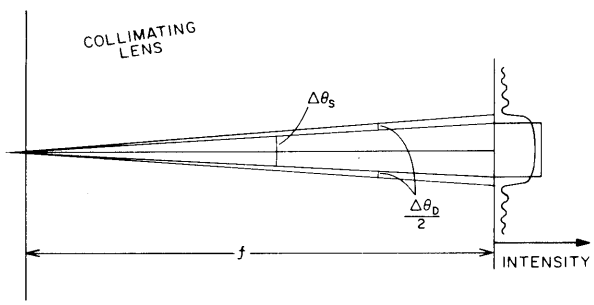

Fig. 4b - Schematic diagram of the angular width of the monochromator image of a finite entrance slit on the exit slit

diffraction is related to the width of the diffraction maximum and can be written as a function of α. A convenient method of writing $\Delta\theta_D$ is

$$\Delta\theta_D = \frac{\lambda}{D} h(\alpha), \tag{4}$$

where $h(\alpha)$ is a function (to be discussed in a later section) which when multiplied by λ/D gives the extension to the angular width due to diffraction. Hence

$$\Delta\theta = \frac{\lambda}{D}\left[\alpha + h(\alpha)\right]. \tag{5}$$

The spectral wavelength range associated with this total angular width can be expressed as

$$\Delta\lambda = \frac{\Delta\lambda}{\Delta\theta}\Delta\theta = \frac{D\Delta\theta}{D\frac{\Delta\theta}{\Delta\lambda}} = D\frac{\Delta\theta}{R_0}, \tag{6}$$

where

$$R_0 = D\frac{\Delta\theta}{\Delta\lambda} = \frac{\lambda}{\Delta\lambda}\left[\alpha + h(\alpha)\right]. \tag{7}$$

Equation (7) may be rewritten as

$$\frac{\lambda}{\Delta\lambda} = \frac{R_0}{\left[\alpha + h(\alpha)\right]}, \tag{8}$$

which serves to illustrate the significance of the various parameters. The factor R_0 is the usual definition of resolution in terms of diffraction patterns and the Rayleigh criterion. When α approaches zero $(S \to 0)$ and $h(\alpha)$ approaches unity,

$$\frac{\lambda}{\Delta\lambda} \to \frac{\lambda}{\delta\lambda} = R_0 , \tag{9}$$

where $\delta\lambda$ is the wavelength separation of two diffraction patterns when the maximum of one falls at the first minimum of the other. In this special case the total angular width is associated with diffraction, and the geometric image of the entrance slit is infinitesimally narrow. However, in practice this situation is not obtained, and the actual or practical resolution R is given by rewriting Eq. (8) as

$$R = \frac{\lambda}{\Delta\lambda} = \frac{R_0}{\left[\alpha + h(\alpha)\right]} = pR_0, \tag{10}$$

where $p = 1/\left[\alpha + h(\alpha)\right]$. The quantity p is called a purity factor by Schuster (7). Then Eq. (10) rewritten gives

$$R = \frac{\lambda}{\Delta\lambda} = pR_0 = p\,\frac{\Delta\theta}{\Delta n}\,\frac{\Delta n}{\Delta\lambda}\,D . \tag{11}$$

To relate the angular dispersion to the prism parameters, we consider the limiting case when

$$\frac{\lambda}{\Delta\lambda} = p\left[\frac{d\theta}{dn}\,\frac{dn}{d\lambda}\right]D = p\,\frac{d\theta}{d\lambda}\,D . \tag{12}$$

The quantity $d\theta/d\lambda$ may be associated with the wavelength interval included in an angular width formed by the exit slit and collimating mirror ignoring diffraction effects. As an example, consider two rays of wavelength λ_0 and $\lambda_0 + d\lambda$ passing through the center of the entrance slit. Assume that λ_0 passes through the prism at the angle of minimum deviation and passes out through the center of the exit slit. The ray $\lambda_0 + d\lambda$ will strike the prism at the same angle of incidence but will be refracted a different amount and, consequently, will pass through the exit slit at a different place. This angular width (associated with an infinitesimal entrance slit) due to slightly different indexes of refraction is the physical bases for $d\theta/d\lambda$. The magnitude of the angular variation with wavelength can be expressed in parameters associated with the prism. Assume as in the previous example that a ray of wavelength λ_0 passes through the center of the entrance slit and that it also passes through the center of the exit slit. Assume that λ_1 and λ_2 are the maximum and minimum wavelength which can pass through the center of the entrance slit and fall in the geometrical image of the entrance slit on the exit slit. Then let $\Delta\lambda = \lambda_1 - \lambda_2$. The angular width associated with this wavelength interval is $\Delta\theta_S = S/f$.

This same wavelength interval could be swept across the slit by an appropriate change in the angle of incidence (rotation of the prism or Littrow mirror). The wavelength interval $\Delta\lambda$ associated with the angular width $\Delta\theta_S$ is related to the way the angle of incidence for minimum deviation changes with wavelength. With use of the symmetry for λ_0 at minimum deviation, Fig. 5 shows how much the angle of incidence i must be changed to sweep λ_1 to to the other side of the exit slit. When the paths of the rays are reversed, λ_1 has an angle of incidence of $i + \Delta\theta_S/2$ and the emergent λ_1 will have an angle of final refraction equal to i. Also, if λ_2 has an angle of incidence of $i - \Delta\theta_S/2$, then the emergent λ_2 will have an angle of final refraction equal to i. Thus the Δi required to make λ_1 go through the other side of the slit is

$$\Delta i = \Delta\theta_S .$$

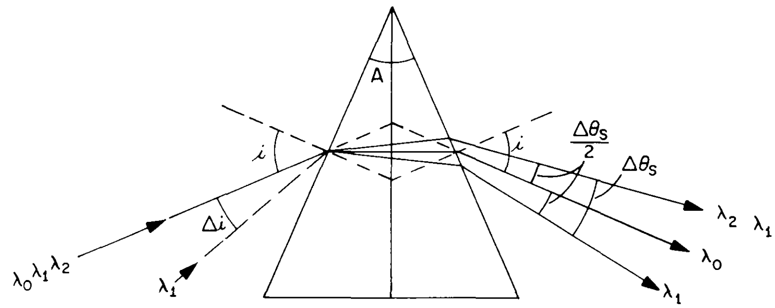

Fig. 5 - Refraction of three wavelengths through a prism

Then

$$\frac{\Delta i}{\Delta n} = \frac{\Delta \theta_S}{\Delta n}.$$

or in the limit

$$\frac{di}{dn} = \frac{d\theta}{dn}$$

where the subscript S has been dropped. We may then write

$$\frac{di}{dn} = \frac{d\theta}{dn} = \frac{2 \sin \frac{A}{2}}{\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}}. \tag{13}$$

This equation, valid at the angle of minimum deviation, is given in most optics books (3). Equation (12) can now be expressed completely in terms of prism parameters, since the dispersion $dn/d\lambda$ is also known.

This discussion was in terms of a single pass through the prism to keep the arguments simple. Since the calculations are to be for a prism used with two passes, the value of $d\theta/dn$ to be substituted into Eq. (12) will be

$$\frac{d\theta}{dn} = \frac{4 \sin \frac{A}{2}}{\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}}. \tag{14}$$

Then Eq. (12) becomes

$$\frac{\lambda}{\Delta\lambda} = p \frac{4 \sin \frac{A}{2}}{\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}} \frac{dn}{d\lambda} D, \tag{15}$$

or the total spectral range of wavelengths $\Delta\lambda$ is

$$\Delta\lambda = \frac{\lambda}{pD\frac{dn}{d\lambda}} \frac{\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}}{4 \sin \frac{A}{2}}. \tag{16}$$

Since

$$\frac{1}{p} = \alpha + h(\alpha) = \frac{SD}{\lambda f} + h(\alpha),$$

then

$$\Delta\lambda = \frac{S}{f\frac{dn}{d\lambda}} \frac{\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}}{4 \sin \frac{A}{2}} + \frac{\lambda\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}}{4D\frac{dn}{d\lambda} \sin \frac{A}{2}} h(\alpha). \tag{17}$$

For purposes of calculation, the collimated beamwidth D can be expressed in terms of b, the width of the prism base. With reference to Fig. 4a

$$\overline{BC} = \frac{b}{2 \sin \frac{A}{2}}.$$

If the angle of minimum deviation is ψ, then

$$i = \frac{A + \psi}{2} \text{ and } n = \frac{\sin \frac{A+\psi}{2}}{\sin \frac{A}{2}}.$$

Also,

$$D = \overline{BC} \cos i = \overline{BC}\left(1 - \sin^2 i\right)^{1/2}$$

$$= \overline{BC}\left(1 - \sin^2 \frac{A+\psi}{2}\right)^{1/2} = \overline{BC}\left(1 - \frac{\sin^2 \frac{A}{2}}{\sin^2 \frac{A}{2}} \sin^2 \frac{A+\psi}{2}\right)^{1/2}$$

$$= \overline{BC}\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2} = \frac{b}{2 \sin \frac{A}{2}}\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}.$$

This expression for D used in Eq. (17) yields

$$\Delta\lambda = \frac{S\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}}{f\frac{dn}{d\lambda} 4 \sin \frac{A}{2}} + \frac{\lambda}{2b\frac{dn}{d\lambda}} h(\alpha)$$

$$= \Delta\lambda_S + \Delta\lambda_P' h(\alpha)$$

$$= \Delta\lambda_S + \Delta\lambda_P. \tag{18}$$

In wave numbers the results are

$$\Delta\nu = \frac{S\left(1 - n^2 \sin^2 \frac{A}{2}\right)^{1/2}}{f \frac{dn}{d\nu} 4 \sin \frac{A}{2}} + \frac{1}{2\nu b \frac{dn}{d\nu}} h(\alpha)$$

$$= \Delta\nu_S + \Delta\nu_P' h(\alpha)$$

$$= \Delta\nu_S + \Delta\nu_P. \tag{19}$$

The first term on the right is associated with the spectral resolution due to finite slit width, while the second term is associated with the prism resolution due to diffraction caused by limiting the optical beam to a width D. Note that with two passes, we neglect slight changes in the beamwidth and "effective" prism base such as are discussed by Cross and Nixon (6).

PRISM RESULTS

The two terms in Eqs. (18) and (19) have been calculated for the prisms listed in Table 1. The results are shown at the end of the report in Figs. 11-18 in wave numbers rather than wavelength. The term $\Delta\nu_S$ was calculated for $S = 0.01$ cm. The results are plotted as $\Delta\nu_S$ vs ν. The term $\Delta\nu_P'$ was calculated and the results plotted as $\Delta\nu_P'$ vs ν. The complete second term $\Delta\nu_P$ may be obtained after $h(\alpha)$ is determined graphically using Fig. 9. In many practical cases with wide slits, $\Delta\nu_P'$ is negligible compared to $\Delta\nu_S$ and even more negligible when the value of $h(\alpha)$ is considered.

DISCUSSION OF $h(\alpha)$

The quantity $h(\alpha)$ is contained in the purity factor p and has been calculated by Schuster (7). In his treatment the physical slit width is measured in units of $\alpha = SD/f\lambda$. For a very narrow entrance slit with $\alpha = 0$ as shown in Fig. 6, the first diffraction minimum occurs at a distance ϵ from the center of the diffraction pattern. At $\epsilon/2$ the intensity has dropped to 0.405 of the maximum intensity. For an entrance slit of finite width α, the distance from the center at which the intensity is 0.405 is determined. Twice this distance is called the "distance of resolution." The reciprocal of this distance is called the purity factor p. It expresses the fraction of the highest possible resolving power (Rayleigh criterion) which is retained with finite slit widths. As can be seen in Fig. 6, when the physical slit width $\alpha = 1$, the geometrical image of the entrance slit has a width ϵ and fills the diffraction pattern for an infinitesimal entrance slit out to an intensity of 0.405. The actual image of the finite entrance slit is wider than ϵ. The width out to an intensity of 0.405 is $1/p = 1.283$, which means that the Rayleigh resolving power is not quite reached. The actual resolving power R is then given as $R = pR_0 = 0.779\ R_0$, where R_0 is the Rayleigh resolving power. In Fig. 9 are shown plots of α vs $1/p$ and α vs $h(\alpha)$ based on the calculations of Schuster.

In most practical cases, the value of α used is larger than 2, so that the spectral slit width term $\Delta\nu_P = \Delta\nu_P'\ h(\alpha)$ is negligible compared to $\Delta\nu_S$ since $h(\alpha) \approx 0.2$. As previously noted $\Delta\nu_P'$ is already negligible compared to $\Delta\nu_S$ in many practical cases.

In Fig. 10 is given a plot of S vs λ showing lines of constant α when $D = 5$ cm and $f = 27$ cm. This is useful to determine whether or not $h(\alpha)$ is significant in Fig. 9. A later section will consider a typical example in which use will be made of Figs. 9 and 10.

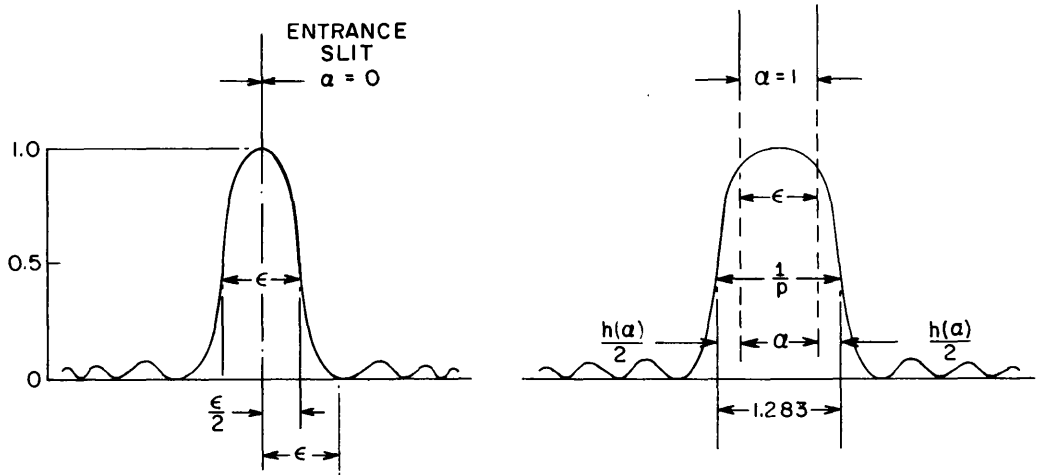

Fig. 6 - Diffraction patterns for infinitesimal and finite physical slit widths

GRATING CALCULATIONS

Equation (12) is general, and for a grating we must merely interpret $d\theta/d\lambda$ in terms of the grating angle ϕ. The optical ray diagram for the grating is shown in Fig. 7, except that a lens instead of a mirror is used for simplicity. At the central image position, $\phi = 0$; at the blaze position, ϕ = blaze angle. We consider $d\theta/d\lambda$ in terms of the angular separation of two wavelengths.

The grating equation with reference to Fig. 7 is given as

$$m\lambda = d(\sin i + \sin \mathcal{D}), \tag{20}$$

where m is the order, d is the grating space, i is the angle of incidence, and $\mathcal{D}$ is the angle of diffraction. In terms of the grating angle ϕ

$$m\lambda = d\left[\sin\left(\phi + \frac{\delta}{2}\right) + \sin\left(\phi - \frac{\delta}{2}\right)\right] = 2d \cos\frac{\delta}{2} \sin \phi, \tag{21}$$

where δ is the angular separation of the entrance and exit slits. For the Perkin-Elmer monochromator $\delta \approx 4$ degrees. Usually $1/(2d \cos \delta/2)$ is defined as K, the grating constant, so that in wave numbers

$$\nu = mK \csc \phi. \tag{22}$$

We are interested in what wavelength interval $\Delta\lambda$ appears across the exit slit (ignoring diffraction). Consider the grating set at an angle ϕ, so that the wavelength λ_0 falls at the center of the exit slit for infinitesimal entrance slit as shown in Fig. 8. Two wavelengths λ_1 and λ_2 fall as the edges of the finite exit slit. The angular separation of λ_1 and λ_2 is considered to be $\Delta\theta_S$. It follows that $i_0 = i_1 = i_2 = \phi + \delta/2$; $\mathcal{D}_0 = \phi - \delta/2$; $\mathcal{D}_1 = \phi - \delta/2 + \Delta\theta_S/2$ and $\mathcal{D}_2 = \phi - \delta/2 - \Delta\theta_S/2$. Then

$$m\lambda_0 = d\left[\sin\left(\phi + \frac{\delta}{2}\right) + \sin\left(\phi - \frac{\delta}{2}\right)\right] \tag{23a}$$

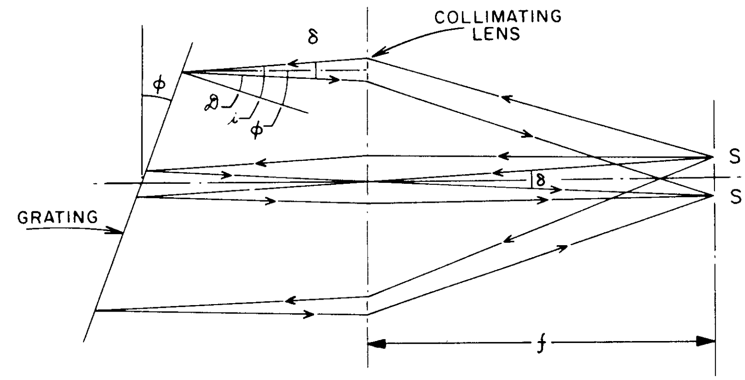

Fig. 7 - Schematic ray diagram for a grating

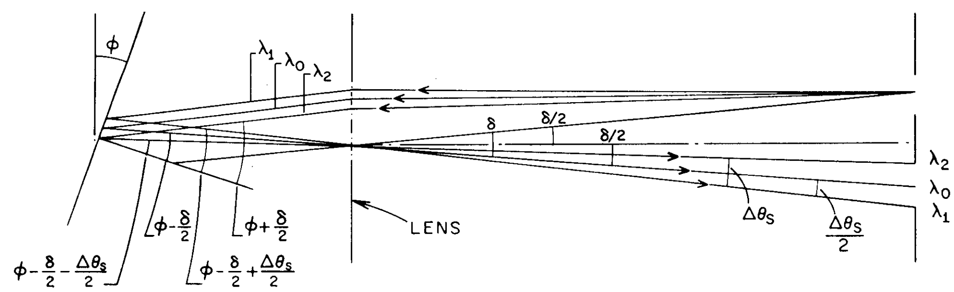

Fig. 8 - Schematic ray diagram for three wavelengths which pass through the middle and edges of the exit slit

$$m\lambda_1 = d\left[\sin\left(\phi + \frac{\delta}{2}\right) + \sin\left(\phi - \frac{\delta}{2} + \frac{\Delta\theta_S}{2}\right)\right] \tag{23b}$$

$$m\lambda_2 = d\left[\sin\left(\phi + \frac{\delta}{2}\right) + \sin\left(\phi - \frac{\delta}{2} - \frac{\Delta\theta_S}{2}\right)\right] \tag{23c}$$

Subtracting Eq. (23c) from Eq. (23b) and defining $\Delta\lambda = \lambda_1 - \lambda_2$, we can write

$$\Delta\lambda = \frac{2d}{m}\cos\left(\phi - \frac{\delta}{2}\right)\sin\frac{\Delta\theta_S}{2} \approx d\,\frac{\Delta\theta_S}{m}\cos\frac{\delta}{2}\cos\phi, \tag{24}$$

since if ϕ is not near 90 degrees, $\sin(\Delta\theta_S/2) \approx (\Delta\theta_S/2)$ and $\sin(\delta/2) \approx 0$, which are generally reasonable working conditions. But with the use of the grating equation, Eq. (21), we can rewrite Eq. (24) as

$$\frac{\Delta\lambda}{\Delta\theta_S} = \frac{\lambda}{2}\,\mathrm{ctn}\,\phi. \tag{25}$$

If we now take the limit, dropping the subscript S and considering a general angular separation $\Delta\theta$, Eq. (25) becomes

$$\frac{d\lambda}{d\theta} = \frac{\lambda}{2}\,\mathrm{ctn}\,\phi. \tag{26}$$

But direct differentiation of the grating equation gives

$$\frac{d\lambda}{d\phi} = \frac{2d}{m}\cos\frac{\delta}{2}\cos\phi = \lambda\,\mathrm{ctn}\,\phi. \tag{27}$$

Therefore

$$\frac{d\lambda}{d\theta} = \frac{1}{2}\frac{d\lambda}{d\phi}. \tag{28}$$

Substituting Eq. (28) in Eq. (12) and using the definition of p (see Eq. (10)) and Eq. (27), we get

$$\Delta\lambda = \frac{\lambda}{D\frac{d\theta}{d\lambda}}\left[\alpha + h(\alpha)\right] = \frac{\lambda^2}{2D}\,\text{ctn}\,\phi\left[\alpha + h(\alpha)\right]. \tag{29}$$

This relation must be modified, for as the grating turns, $D\cos(\delta/2)\cos\phi$ becomes the limiting width of the beam. This modified beamwidth must also be used in the expression for α. Then

$$\Delta\lambda = \frac{\lambda^2\,\text{ctn}\,\phi}{2D\cos\frac{\delta}{2}\cos\phi}\;\frac{SD\cos\frac{\delta}{2}\cos\phi}{f\lambda} + \frac{\lambda^2\,\text{ctn}\,\phi\,h(\alpha)}{2D\cos\frac{\delta}{2}\cos\phi}$$

$$= \frac{\lambda S\,\text{ctn}\,\phi}{2f} + \frac{\lambda^2\,h(\alpha)}{2D\cos\frac{\delta}{2}\sin\phi}. \tag{30}$$

Again using the grating equation, Eq. (30) becomes

$$\Delta\lambda = \frac{\lambda S\,\text{ctn}\,\phi}{2f} + \frac{\lambda d}{Dm}\,h(\alpha) = \Delta\lambda_S + \Delta\lambda_G'\,h(\alpha) = \Delta\lambda_S + \Delta\lambda_G, \tag{31}$$

where $Dm/d = R_0$ is the Rayleigh resolution of the grating. In wave numbers

$$\Delta\lambda = \frac{\nu S\,\text{ctn}\,\phi}{2f} + \frac{\nu\,h(\alpha)}{R_0} = \Delta\nu_S + \Delta\nu_G'\,h(\alpha) = \Delta\nu_S + \Delta\nu_G. \tag{32}$$

The first term is the contribution to the spectral slit width due to the physical slits and the second term is the contribution due to the ultimate resolving power of the grating. However, as in the case of the prism, the ultimate resolving power is not reached, since $\Delta\nu_G$ depends on the physical slit width through the term $h(\alpha)$.

GRATING RESULTS

The first term in Eq. (32) has been calculated for the echelette gratings listed in Table 2 for physical slit widths of 0.1, 0.01, 0.001, or 0.0001 cm. The gratings were all 6.4×6.4 cm^2. The results are shown in Figs. 19-44 as $\Delta\nu_S$ vs ν. It is easy to obtain $\Delta\nu_S$ for any physical slit width since $\Delta\nu_S$ is directly proportional to S. For the second term, only $\Delta\nu_G'$ has been calculated, since for practical physical slit widths $h(\alpha)$ is not usually significant. The results are shown as $\Delta\nu_G'$ vs ν. Of course, $h(\alpha)$ may be obtained from Fig. 9 to correct $\Delta\nu_G'$ to $\Delta\nu_G$ whenever necessary. For most experiments in solid state physics $\Delta\nu_G'$ is negligible compared to $\Delta\nu_S$. From the curves for $\Delta\nu_G'$ and $\Delta\nu_S$, if the slits are open about ten times wider than the S indicated, $\Delta\nu_G'$ is negligible. Also shown in the graphs are curves of ϕ vs ν calculated from Eq. (21) or (22) but neglecting the small terms $\cos(\delta/2) = 0.998$.

EXAMPLE

To illustrate the use of the graphs for prism and grating monochromators, we calculate the resolution for a CsI prism used at 35 μ = 285 cm^{-1} and the Bausch and Lomb

30-μ grating used at 35 μ. Typical slit widths for the prism instrument in a magneto-optical experiment like the free carrier Faraday effect in InSb might be $S = 0.08$ cm. Using the values of f and D shown on Fig. 10, the value of $\alpha \approx 4.2$, and from Fig. 9, $h(\alpha) \approx 0.215$. For a CsI prism Fig. 18 gives a value of $\Delta\nu_{0.01} = 1.15\ \text{cm}^{-1}$ and $\Delta\nu_P' = 1.85\ \text{cm}^{-1}$. Then $\Delta\nu = \Delta\nu_S + \Delta\nu_P' h(\alpha) = 8(1.15) + 1.85(0.215) = 9.20 + 0.40 = 9.60\ \text{cm}^{-1}$. For the grating used at 35 μ in the same experiment with the slits still set at 0.08 cm, we find with the use of Figs. 9, 10, and 32 that $h(\alpha) = 0.215$ for $\alpha \approx 4.2$ and that $\Delta\nu_{0.01} = 0.086$ and $\Delta\nu_G' = 0.15$. Then $\Delta\nu = \Delta\nu_S + \Delta\nu_G' h(\alpha) = 8(0.086) + 0.15(0.215) = 0.69 + 0.03 = 0.72\ \text{cm}^{-1}$.

Everything else being equal, the grating used in place of the prism would provide a factor of ~13 improvement in resolution but because of the added dispersion a factor of ~13 reduction in signal (see the next section). Therefore, the slits of the grating monochromator should be opened about a factor of $\sqrt{13} = 3.6$ to 0.288 cm to arrive back at the original prism signal. Then for the grating $\Delta\nu = 8(3.6)0.086 + 0.15(0.21) = 2.48 + 0.03 = 2.51\ \text{cm}^{-1}$. This resolution is still appreciably better than with the prism monochromator. Finally, if the low resolution of 9.6 cm^{-1} is adequate, the slit of the grating monochromator may be further opened by a factor of 3.8 to about 1.1 cm to give a resolution of 9.6 cm^{-1} with the subsequent gain in signal of $3.8^2 = 14.4$.

POWER CONSIDERATIONS

We briefly set down the expression for the power P reaching the detector in terms of the parameters of the optical system (15):

$$P = \epsilon\tau E \left(\frac{c_1\lambda^{-5}}{e^{c_2/\lambda T} - 1}\right)(d\lambda)\ A\Omega, \tag{33}$$

where

ϵ = emissivity of source

τ = transmission of optical system

E = efficiency of dispersion element

$c_1 = 1.77 \times 10^{-12}$ watts/cm^2-ster-cm

$c_2 = 1.432$ cm-°K

A = area of source

L = length of slit (1 cm for the standard monochromator)

S = width of slit

T = absolute temperature of the source

Ω = solid angle of radiation collected from source (matched to $f/4.2$ of the standard monochromator)

λ = wavelength

For both a prism and a grating $A = SL$ determines $d\lambda$, the spectral slit width, so for everything else being fixed except $d\lambda$ and A, it is easy to compare prisms and gratings as to signals to be expected, provided that estimates of τ and E can be made.

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Table 1
Prisms For Which Calculations Have Been Made

Material	Apex angle A (deg)	Base width b (cm)	Fig.
LiF	72	8.8	11
CaF_2	67	7.8	12
NaCl	60	7.5	13
KBr	60	7.5	14
KRS-5	26	2.9	15
CsBr	25	2.6	16
CsBr	50	7.5	17
CsI	25	2.6	18

Table 2
Gratings For Which Calculations Have Been Made (Area of Gratings, 6.4 × 6.4 cm^2)

Manufacturer	1/d (grooves/cm)	Blaze λ (μ)	Blaze angle	Fig.
Bausch & Lomb	18000	0.50	26°45'	19
Bausch & Lomb	12000	0.75	26°45'	20
Bausch & Lomb	3000	1.2	10°25'	21
Bausch & Lomb	4000	1.6	18°32'	22
Bausch & Lomb	6000	1.6	26°45'	23
Bausch & Lomb	2000	1.7	10°00'	24
Bausch & Lomb	3000	3.0	26°45'	25
Bausch & Lomb	1500	4.0	17°27'	26
Bausch & Lomb	1500	6.0	26°45'	27
Bausch & Lomb	750	8.0	17°27'	28
Bausch & Lomb	750	12.0	26°45'	29
Bausch & Lomb	600	16.0	28°41'	30
Bausch & Lomb	400	20.0	23°35'	31
Bausch & Lomb	300	30.0	26°45'	32
U. of Michigan	219 (556/in.)	40	26°	33
Bausch & Lomb	200	45.0	26°45'	34
U. of Michigan	126 (320/in.)	70	26°	35
U. of Michigan	50.4 (128/in.)	70	10°	36
Bausch & Lomb	100	90	26°45'	37
Bausch & Lomb	80	112.5	26°45'	38
Bausch & Lomb	50	180	26°45'	39
U. of Michigan	39.4 (100/in.)	200	23°12'	40
Bausch & Lomb	40	225	26°45'	41
Farrand	19.7 (50/in.)	347	20°	42
Bausch & Lomb	20	450	26°45'	43
Farrand	9.85 (25/in.)	694	20°	44

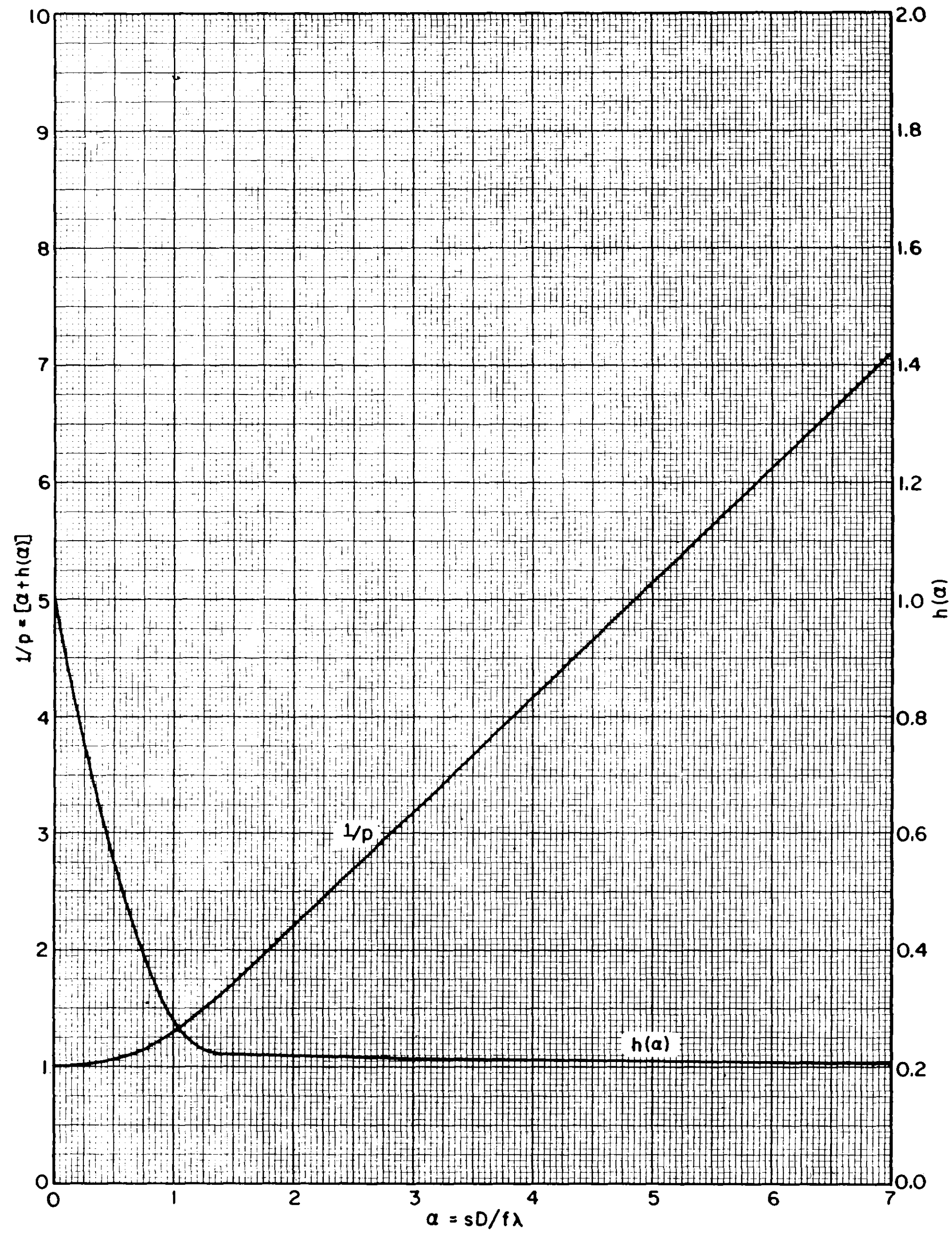

Fig. 9 - Graph of $h(\alpha)$ and $1/p$ vs α based on the calculations of Schuster (7)

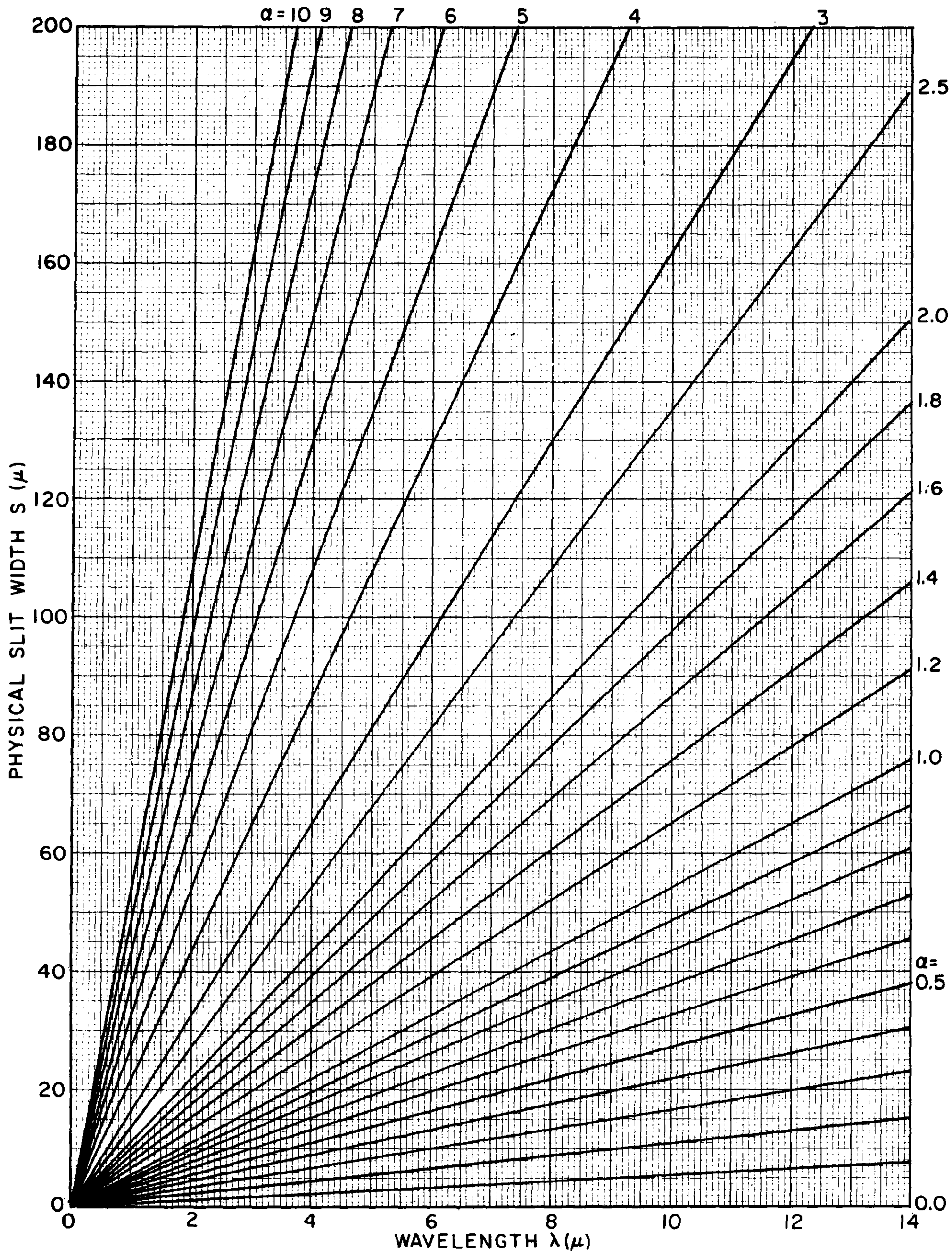

Fig. 10 - Graph of α as a function of physical slit width S and wavelength λ. [$S = (f/D)\alpha\lambda$; for f = 27 cm and D = 5 cm, $S = 5.4\alpha\lambda$.]

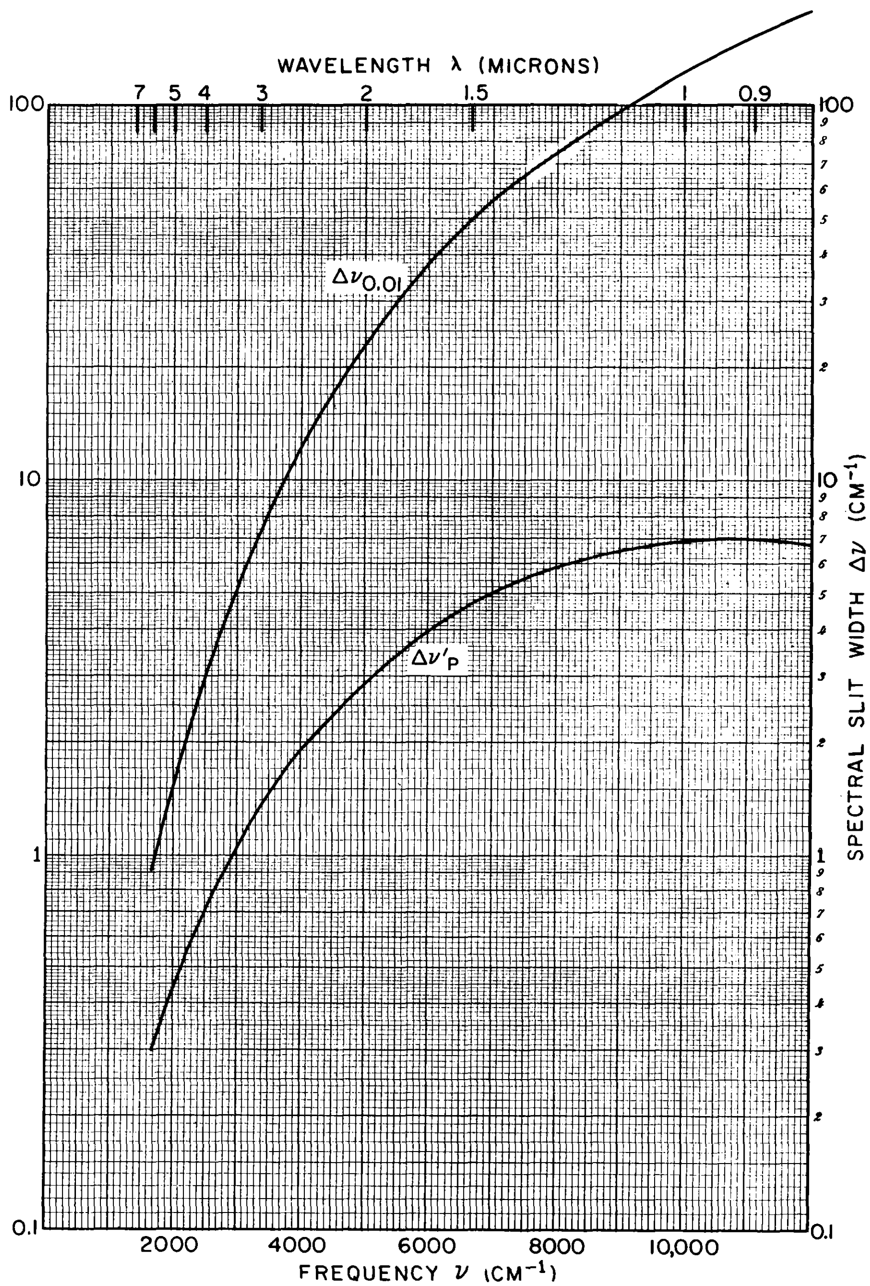

Fig. 11 - Resolution of a LiF prism with A = 72 degrees and b = 8.8 cm (see Table 1)

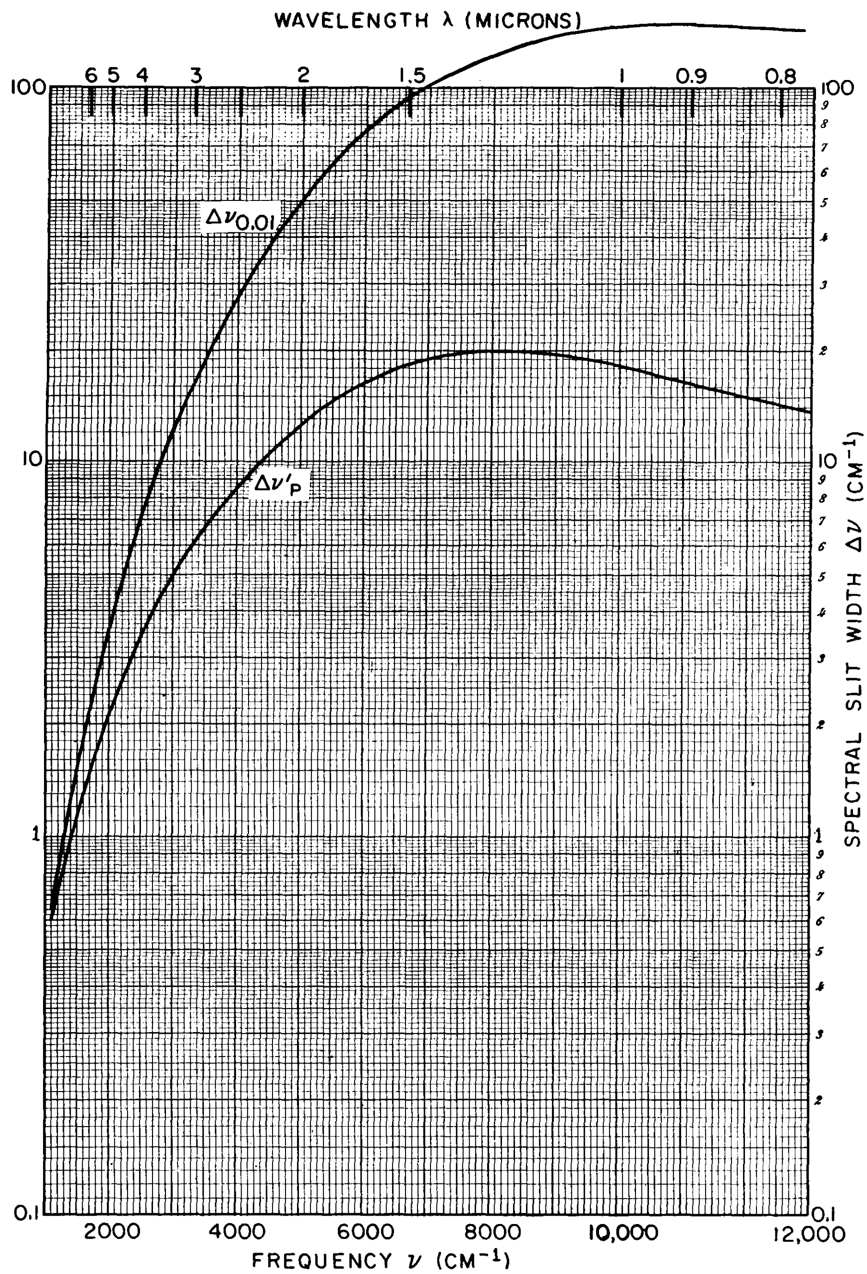

Fig. 12 - Resolution of a CaF_2 prism with A = 67 degrees and b = 7.8 cm

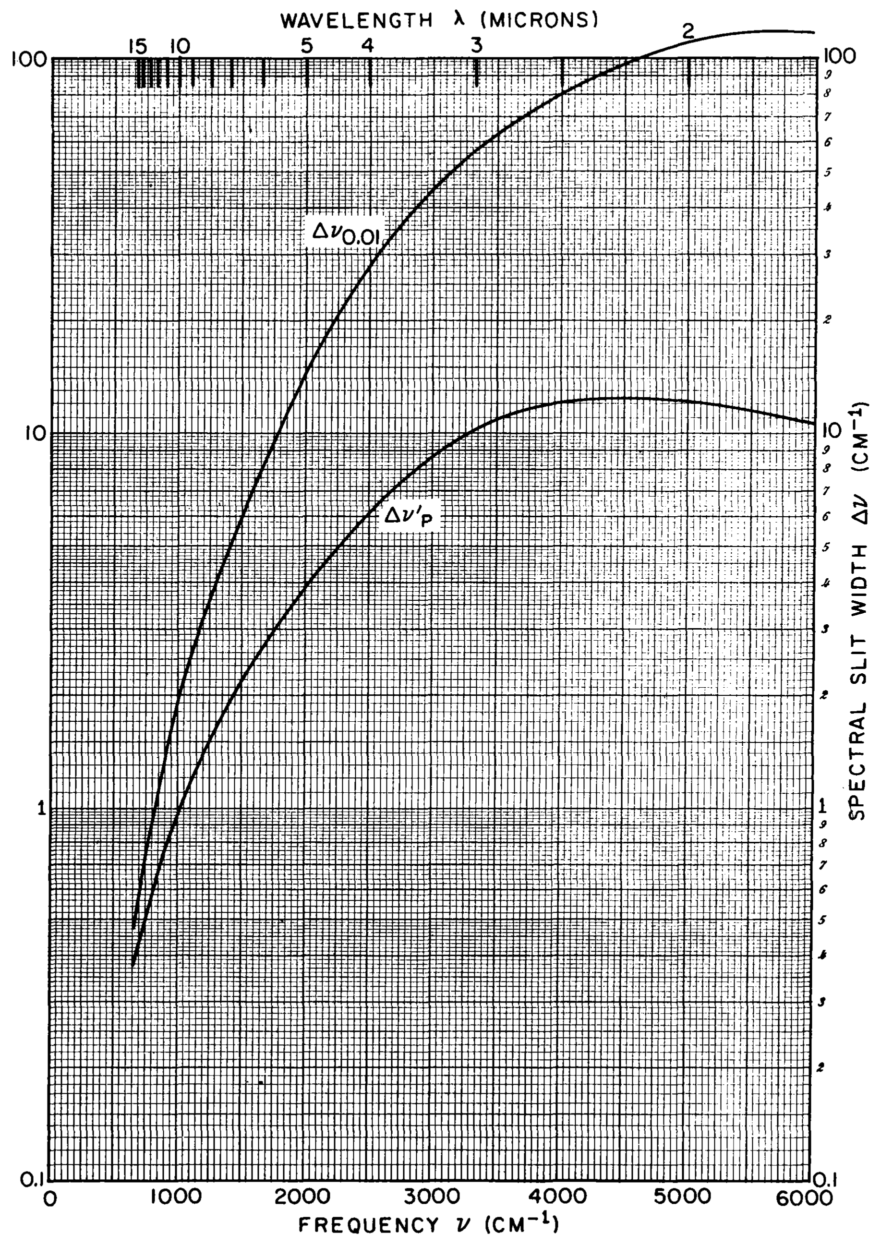

Fig. 13 - Resolution of a NaCl prism with A = 60 degrees and b = 7.5 cm

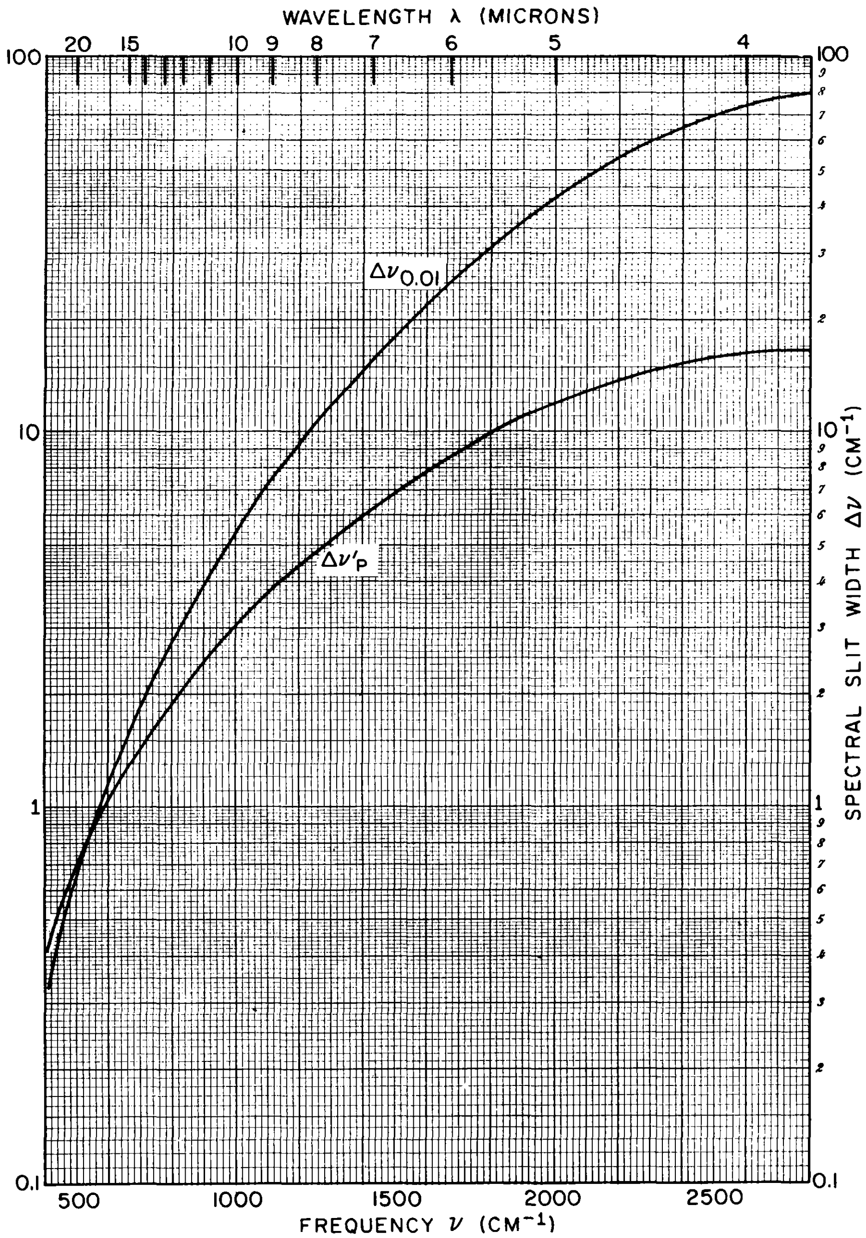

Fig. 14 - Resolution of a KBr prism with A = 60 degrees and b = 7.5 cm

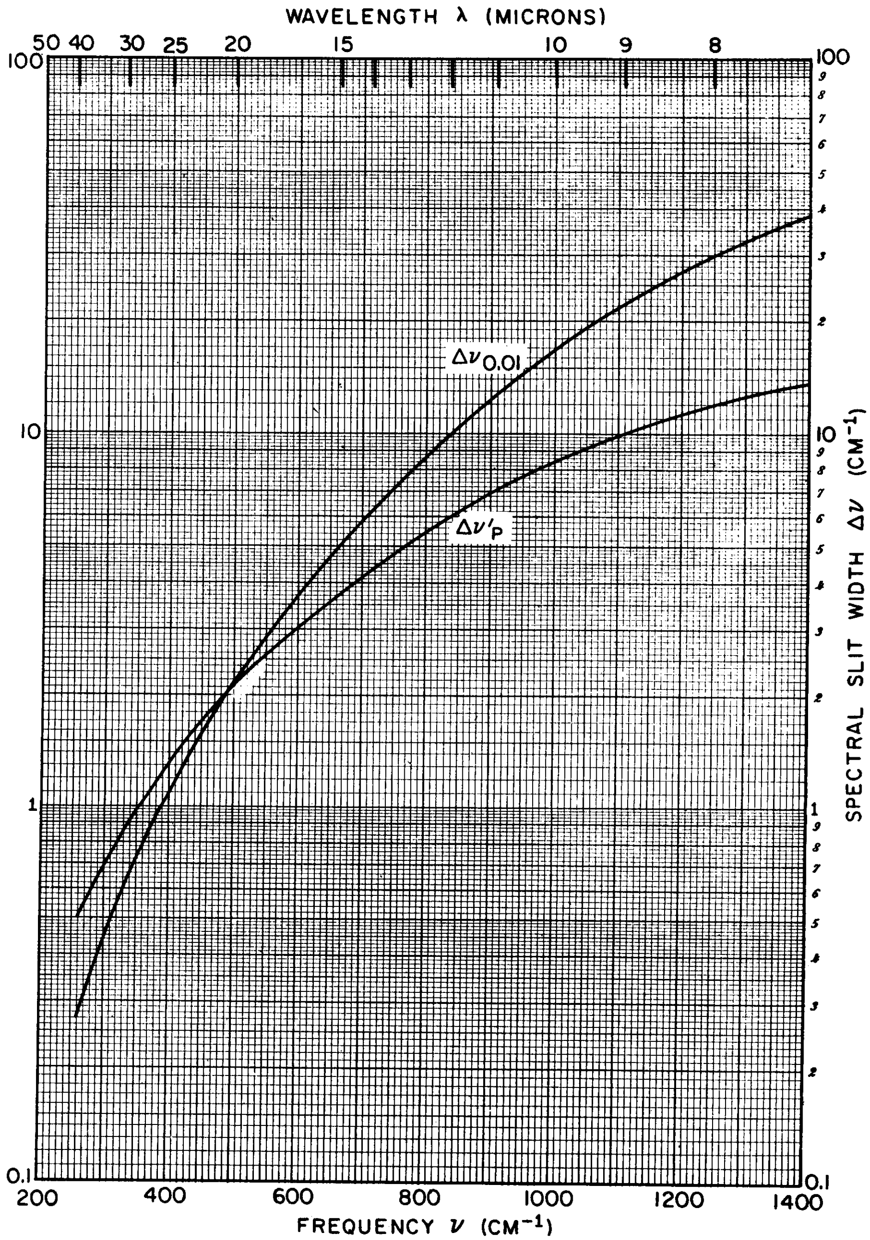

Fig. 15 - Resolution of KRS-5 prism with A = 26 degrees and b = 2.9 cm

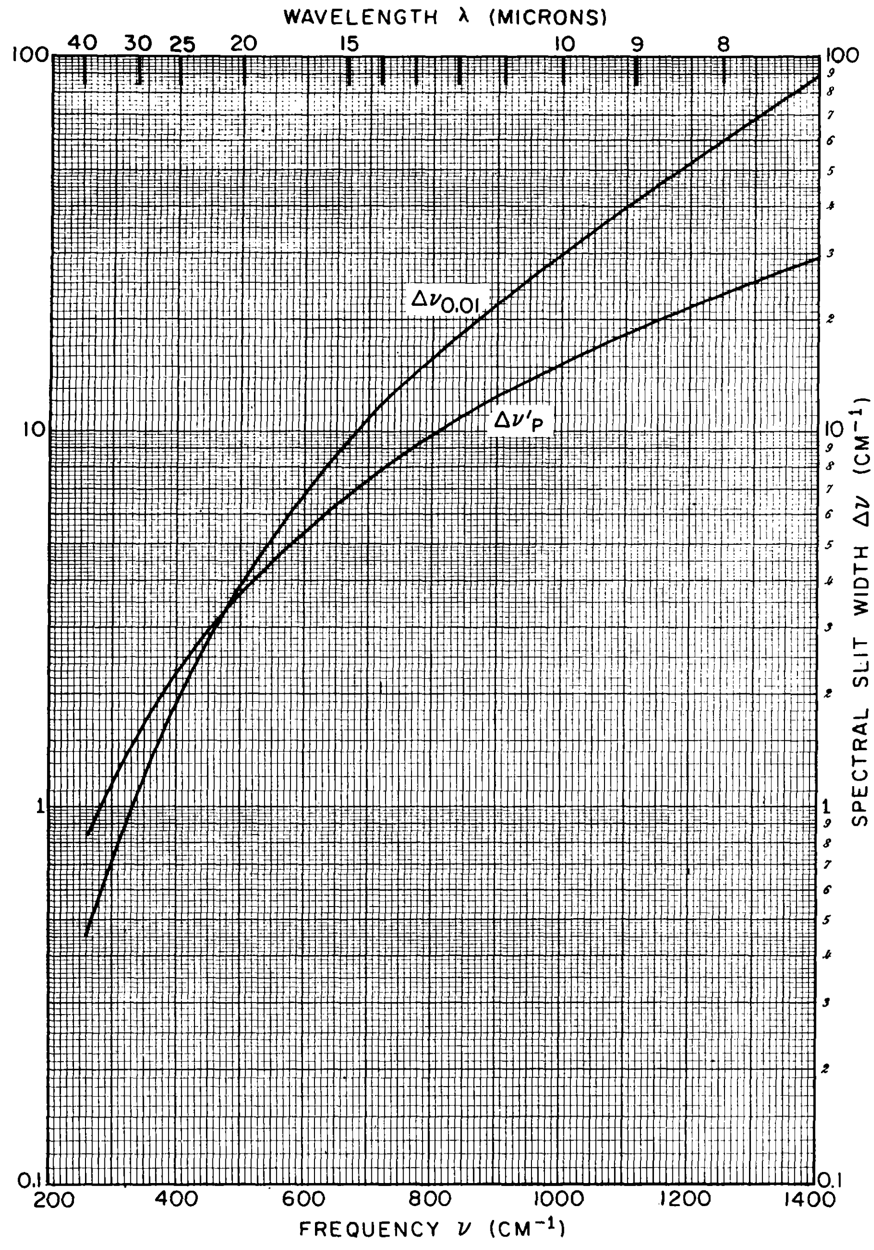

Fig. 16 - Resolution of a CsBr prism with A = 25 degrees and b = 2.6 cm

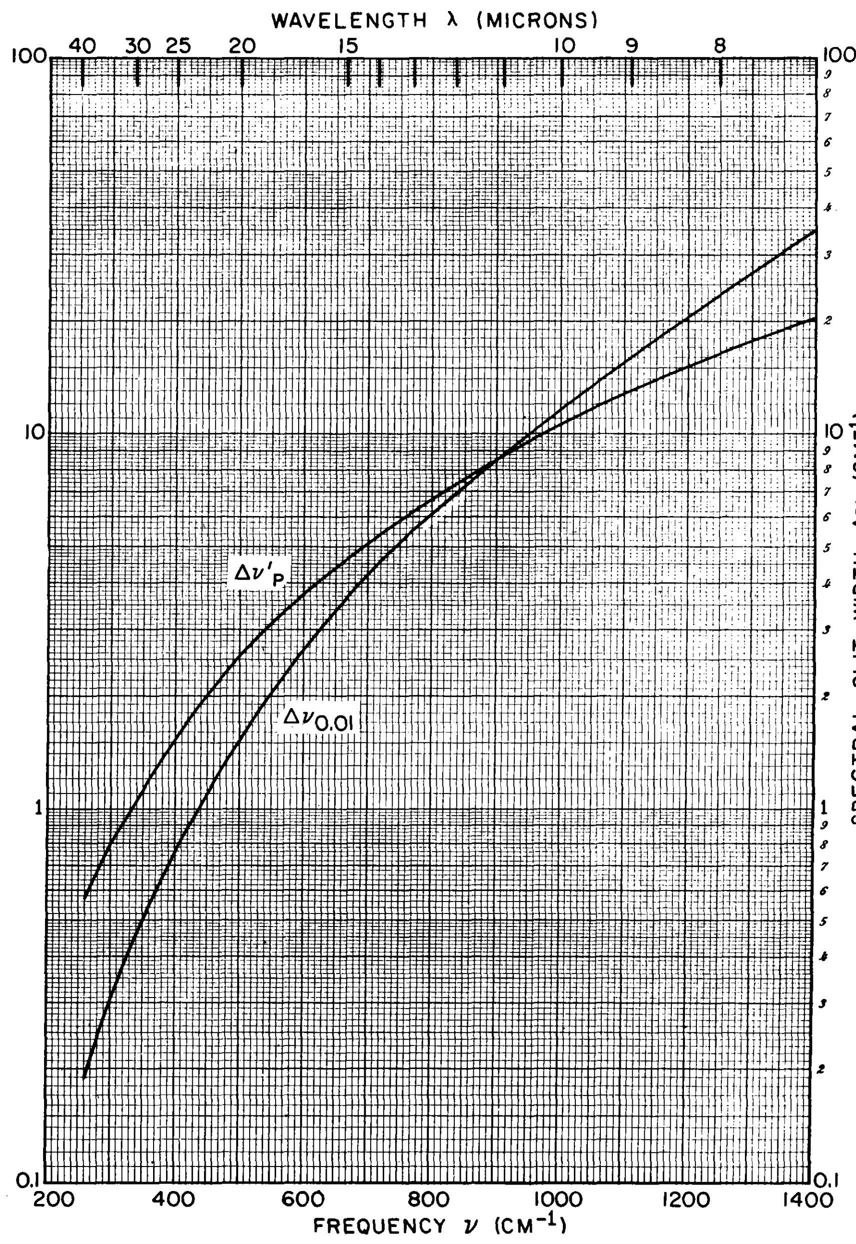

Fig. 17 - Resolution of a CsBr prism with A = 50 degrees and b = 7.5 cm

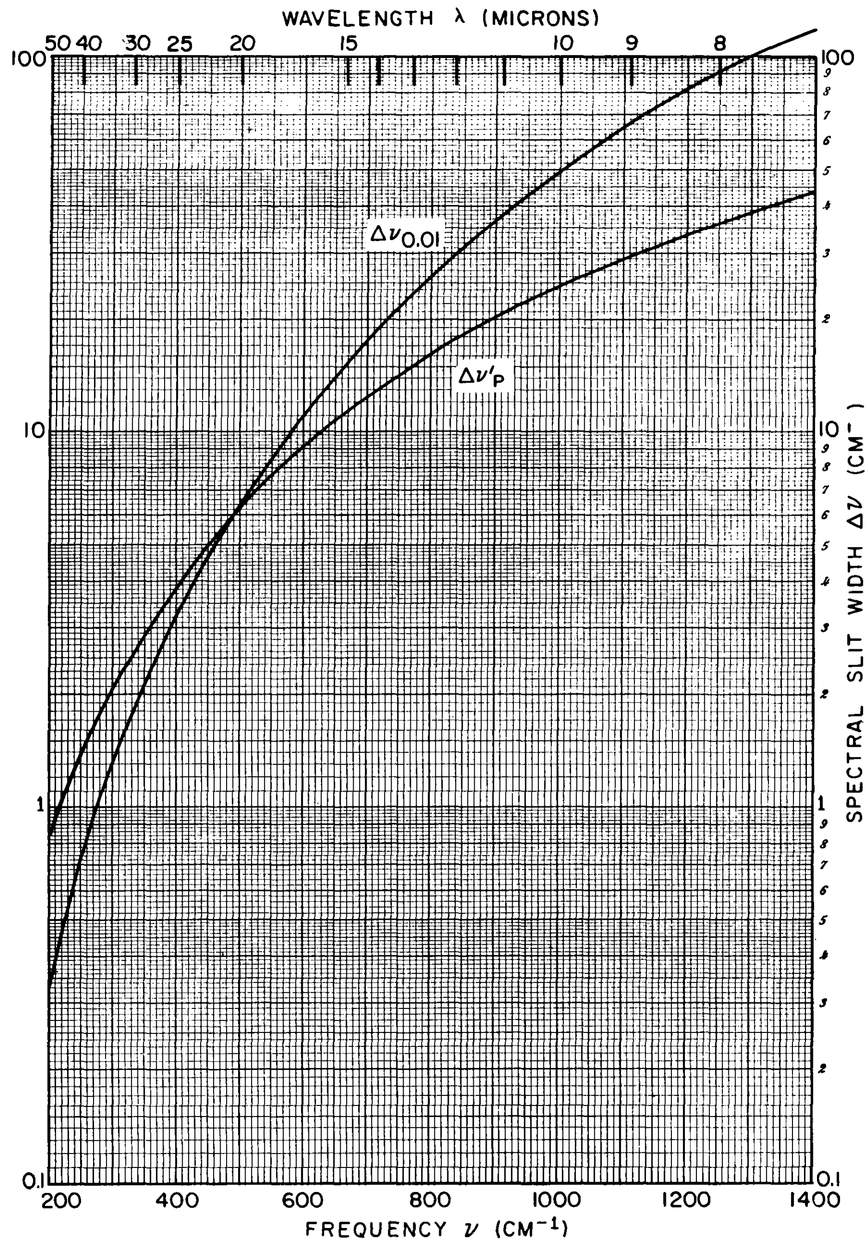

Fig. 18 - Resolution of a CsI prism with A = 25 degrees and b = 2.6 cm

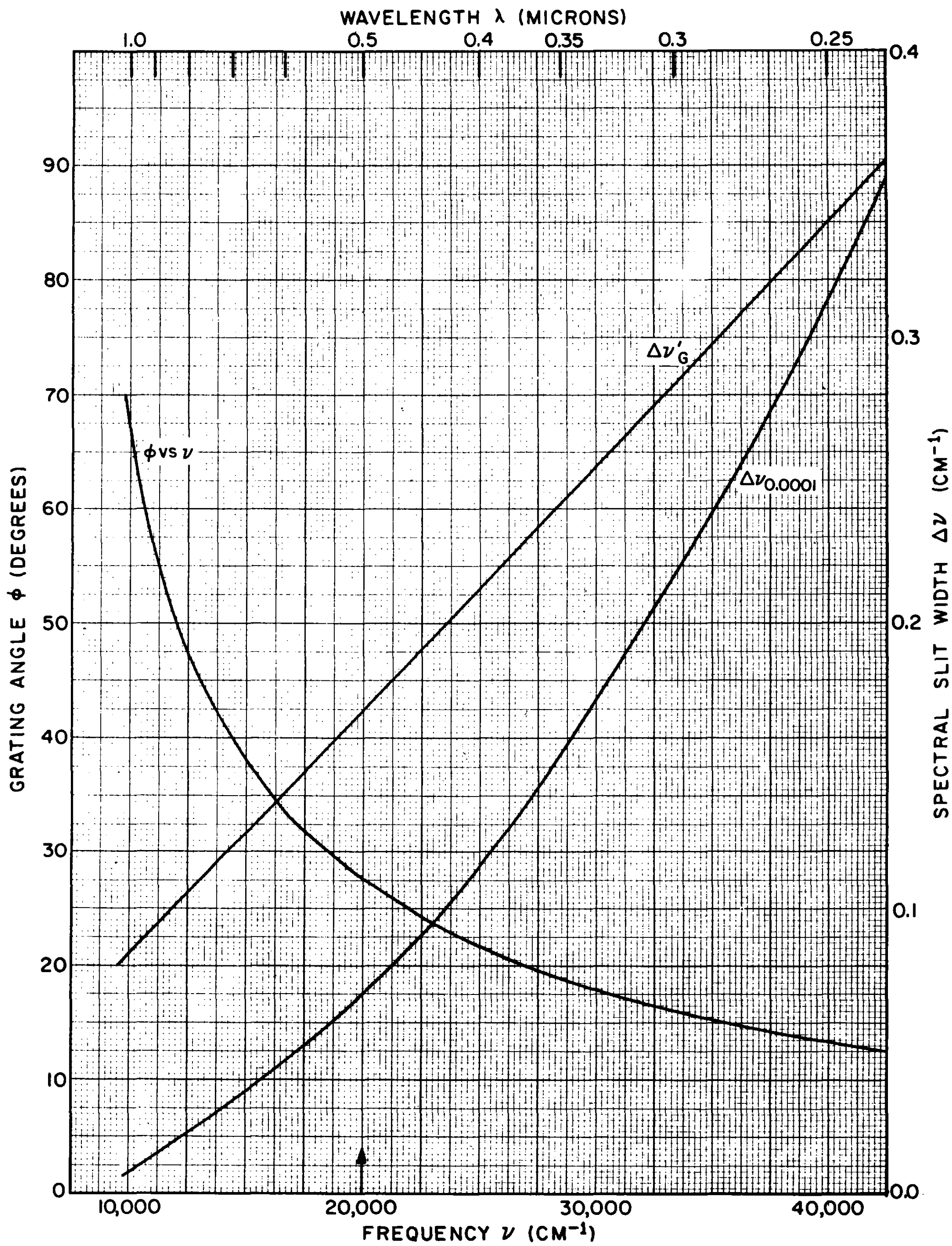

Fig. 19 - Resolution of a grating with a blaze wavelength = 0.50 μ, d = 1/18,000 = 5.55×10^{-5} cm, and R_0 = 117,800

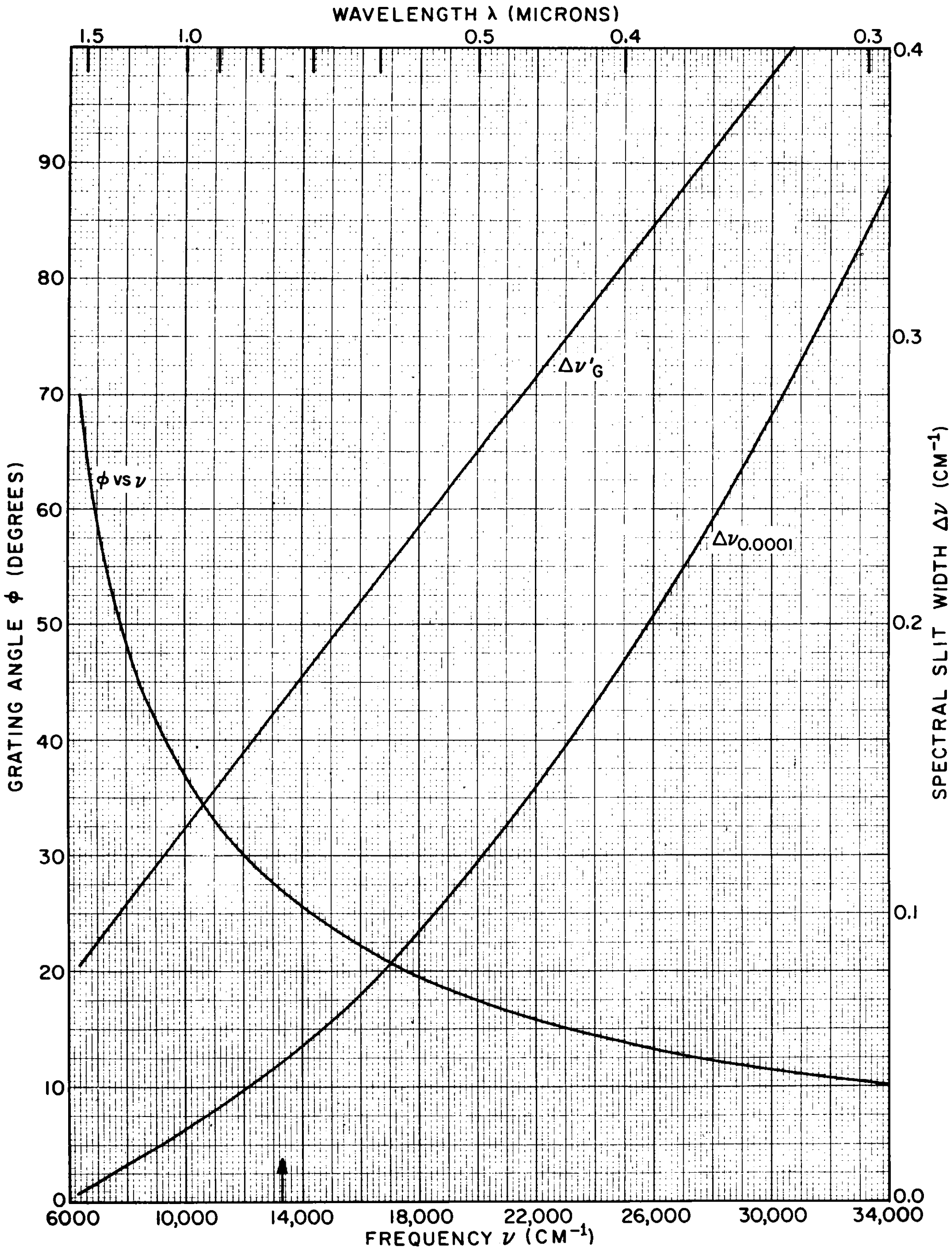

Fig. 20 - Resolution of a grating with a blaze wavelength = 0.75 μ, $d = 1/12{,}000 = 8.34 \times 10^{-5}$ cm, and $R_0 = 76{,}800$

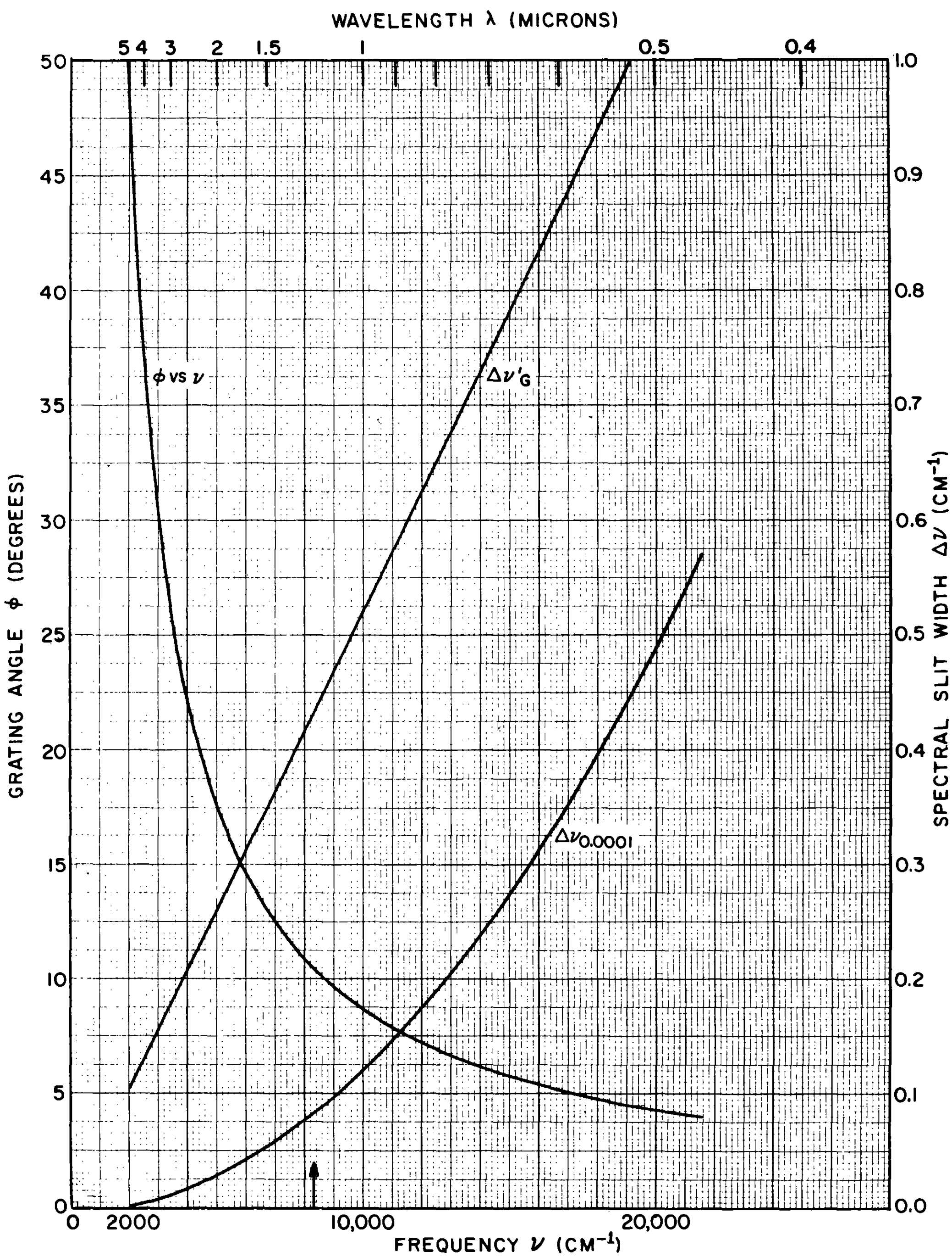

Fig. 21 - Resolution of a grating with a blaze wavelength = 1.2 μ, d = 1/3000 = 3.3×10^{-4} cm, and R_0 = 19,200

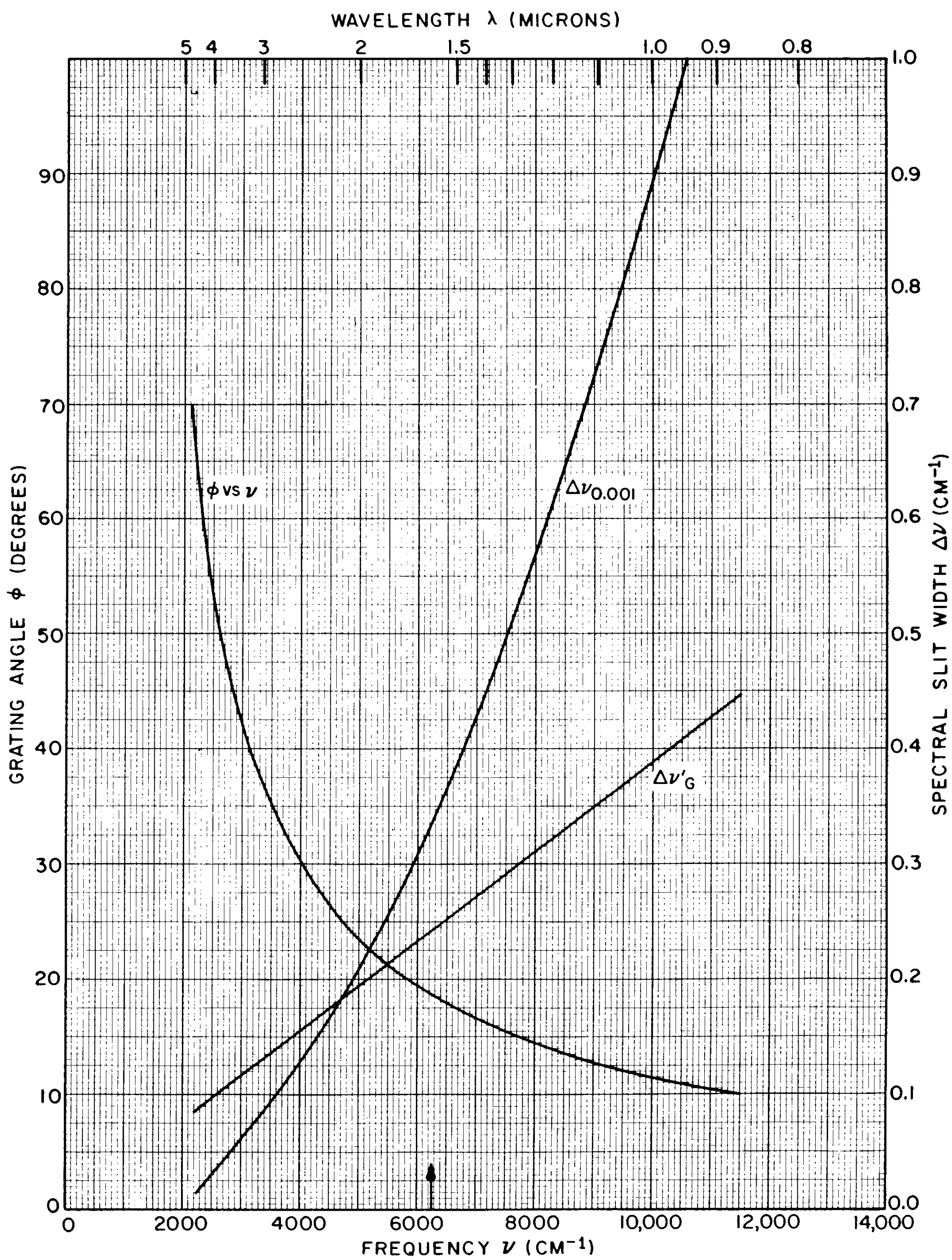

Fig. 22 - Resolution of a grating with a blaze wavelength = 1.6 μ, d = 1/4000 = 2.5×10^{-4} cm, and R_0 = 25,600

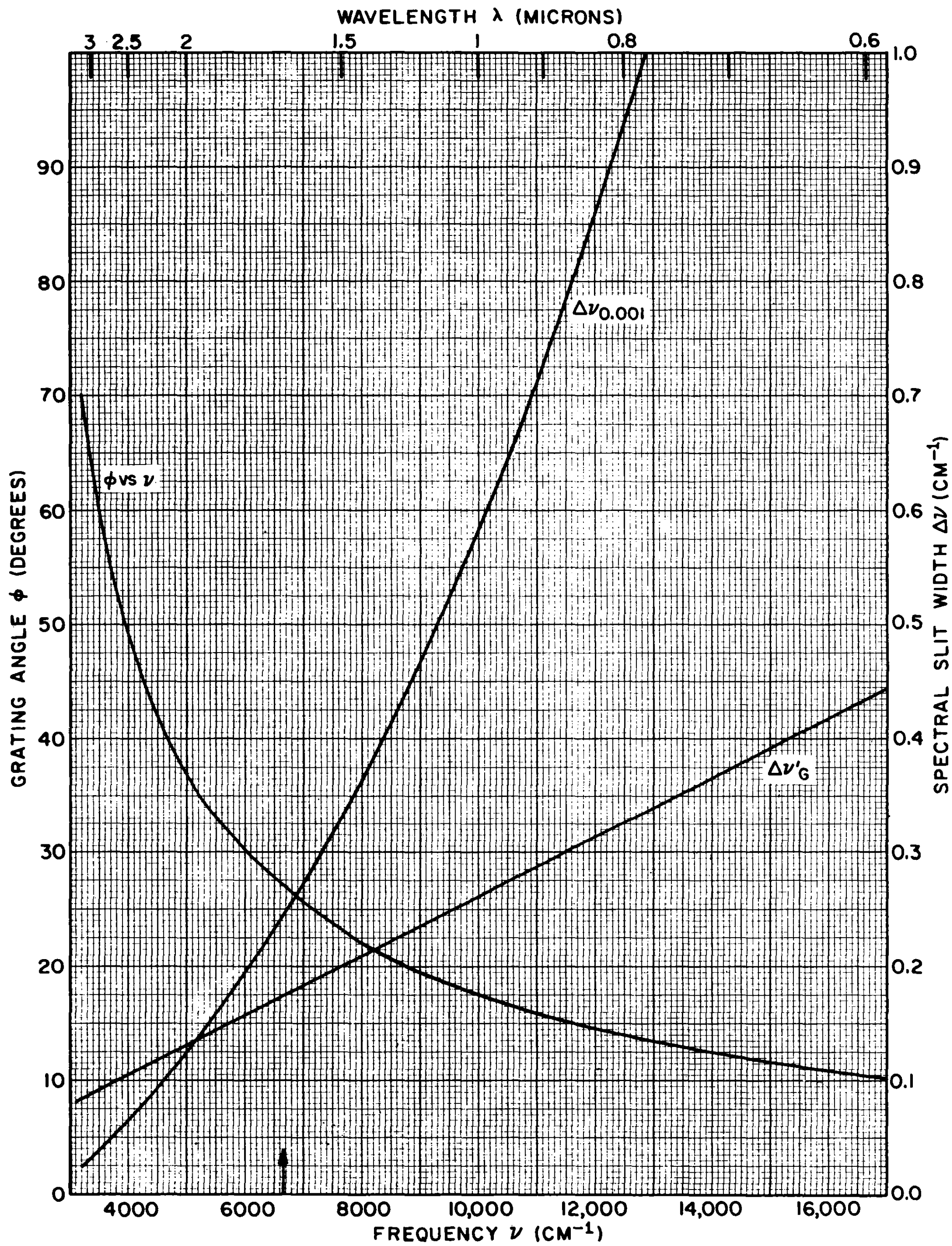

Fig. 23 - Resolution of a grating with a blaze wavelength = 1.6 μ, $d = 1/6000 = 1.66 \times 10^{-4}$ cm, and $R_0 = 38{,}400$

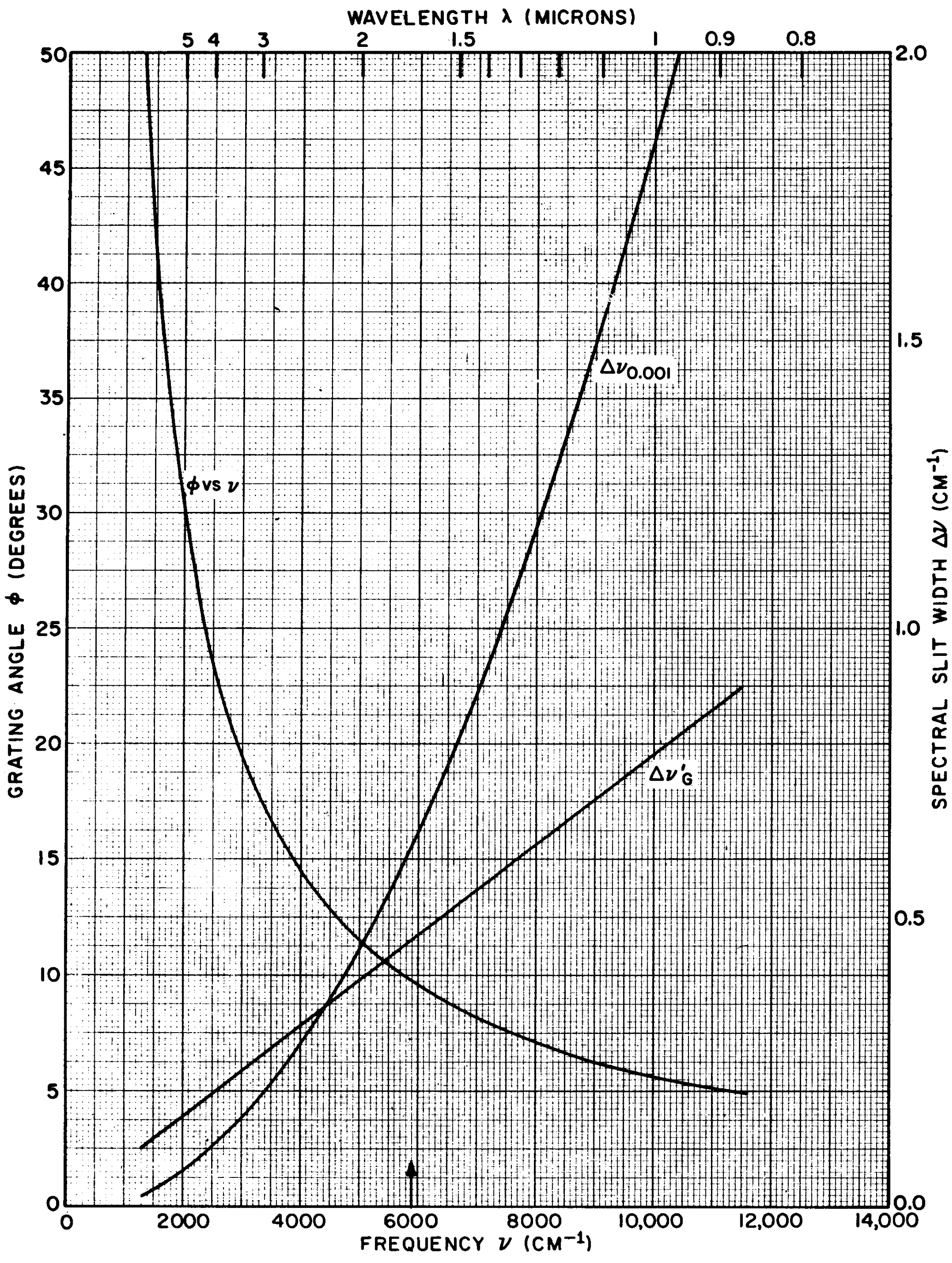

Fig. 24 - Resolution of a grating with a blaze wavelength = 1.7 μ, d = 1/2000 = 5.0 × 10^{-4} cm, and R_0 = 12,800

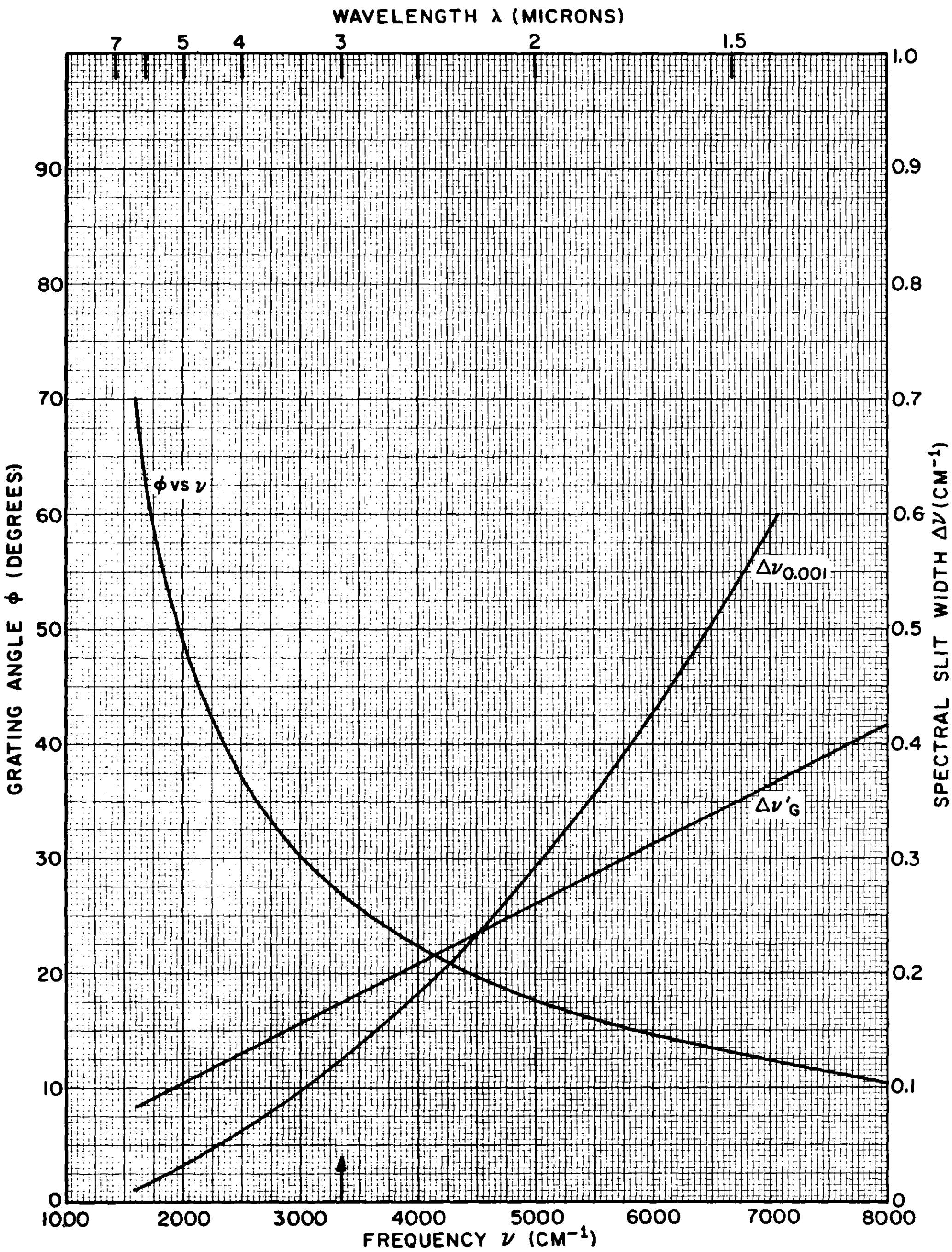

Fig. 25 - Resolution of a grating with a blaze wavelength = 3.0 μ, d = 1/3000 = 3.33×10^{-4} cm. and R_0 = 19,200

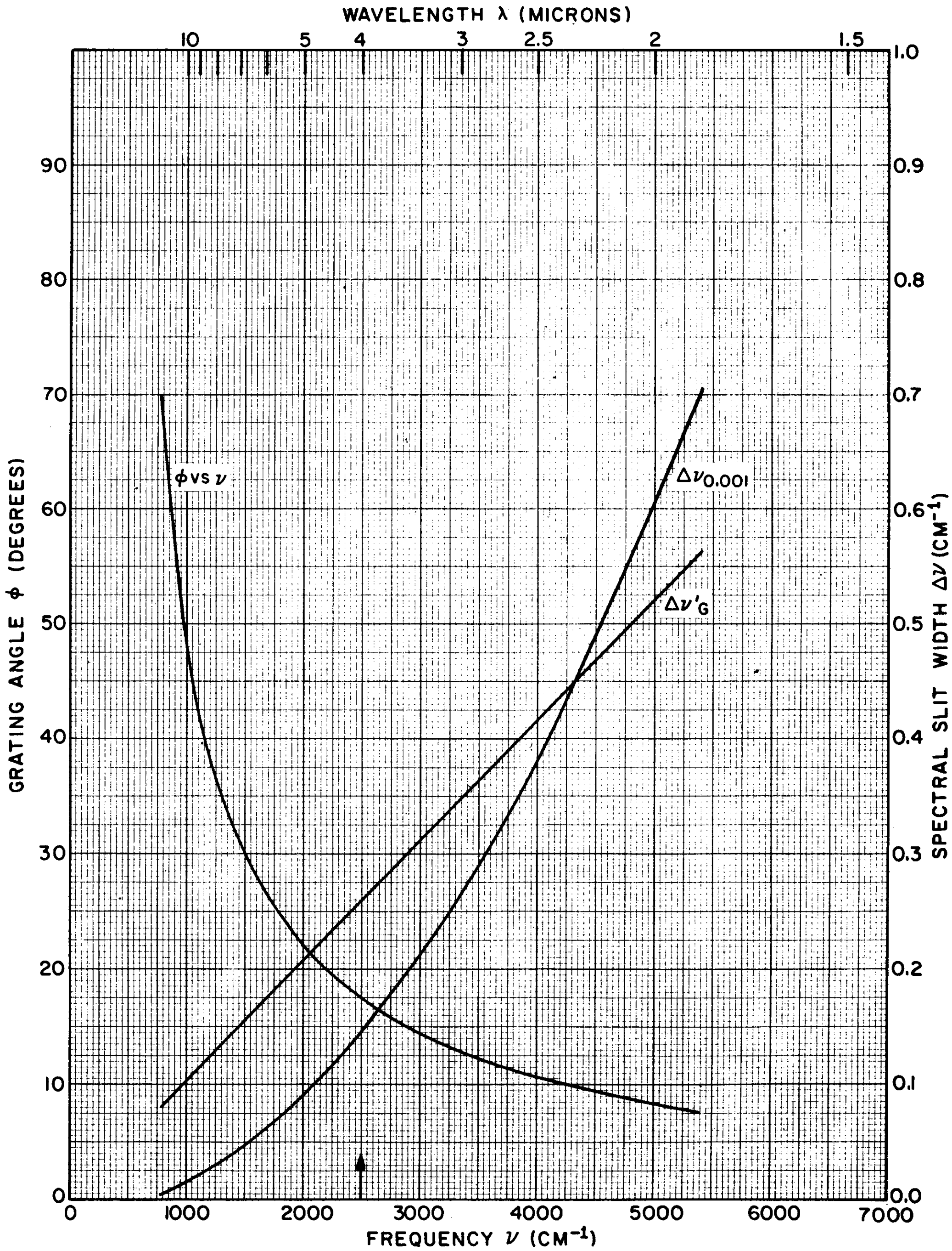

Fig. 26 - Resolution of a grating with a blaze wavelength = 4.0 μ, $d = 1/1500 = 6.66 \times 10^{-4}$ cm, and $R_0 = 9600$

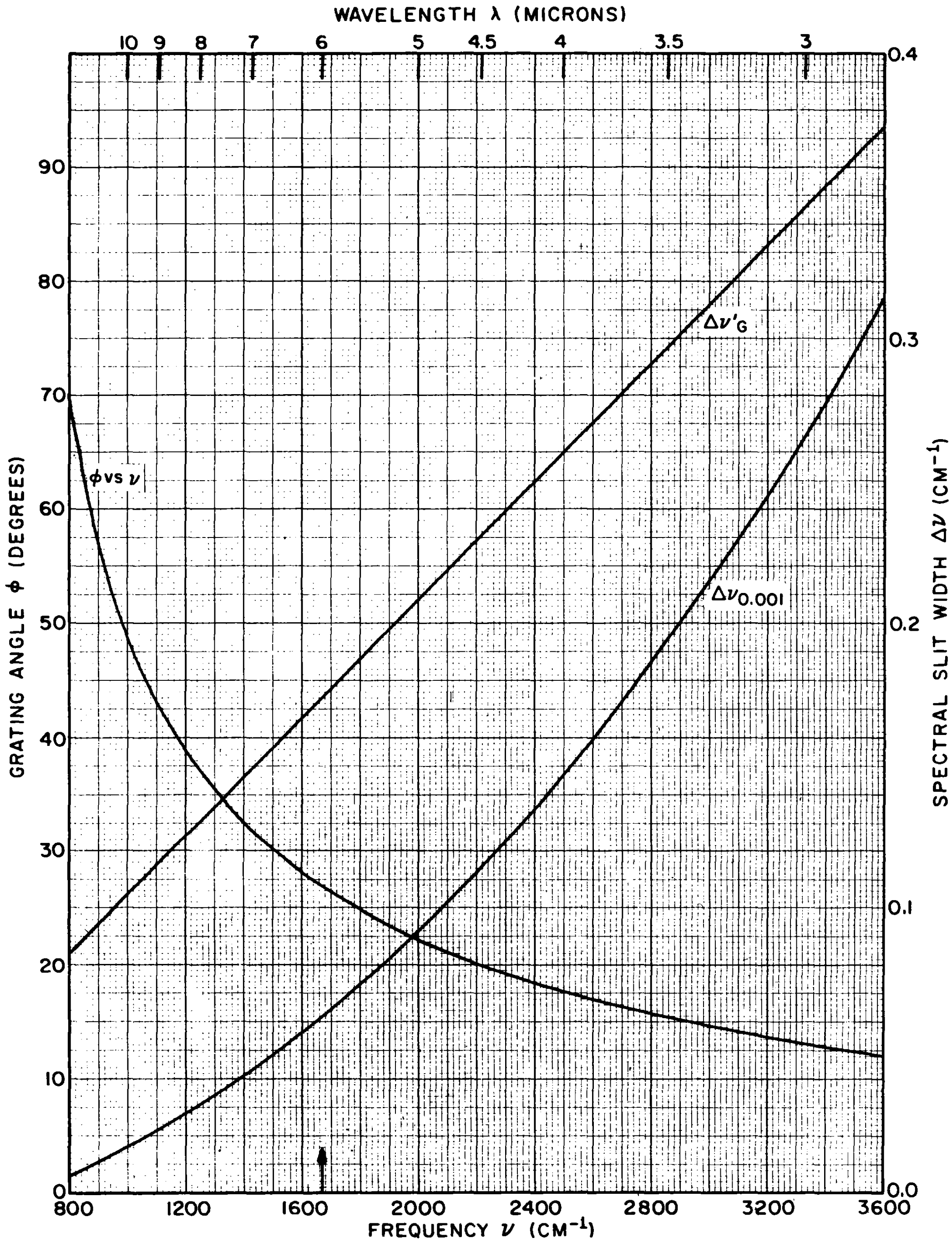

Fig. 27 - Resolution of a grating with a blaze wavelength = 6.0 μ, $d = 1/1500 = 6.66 \times 10^{-4}$ cm, and $R_0 = 9600$

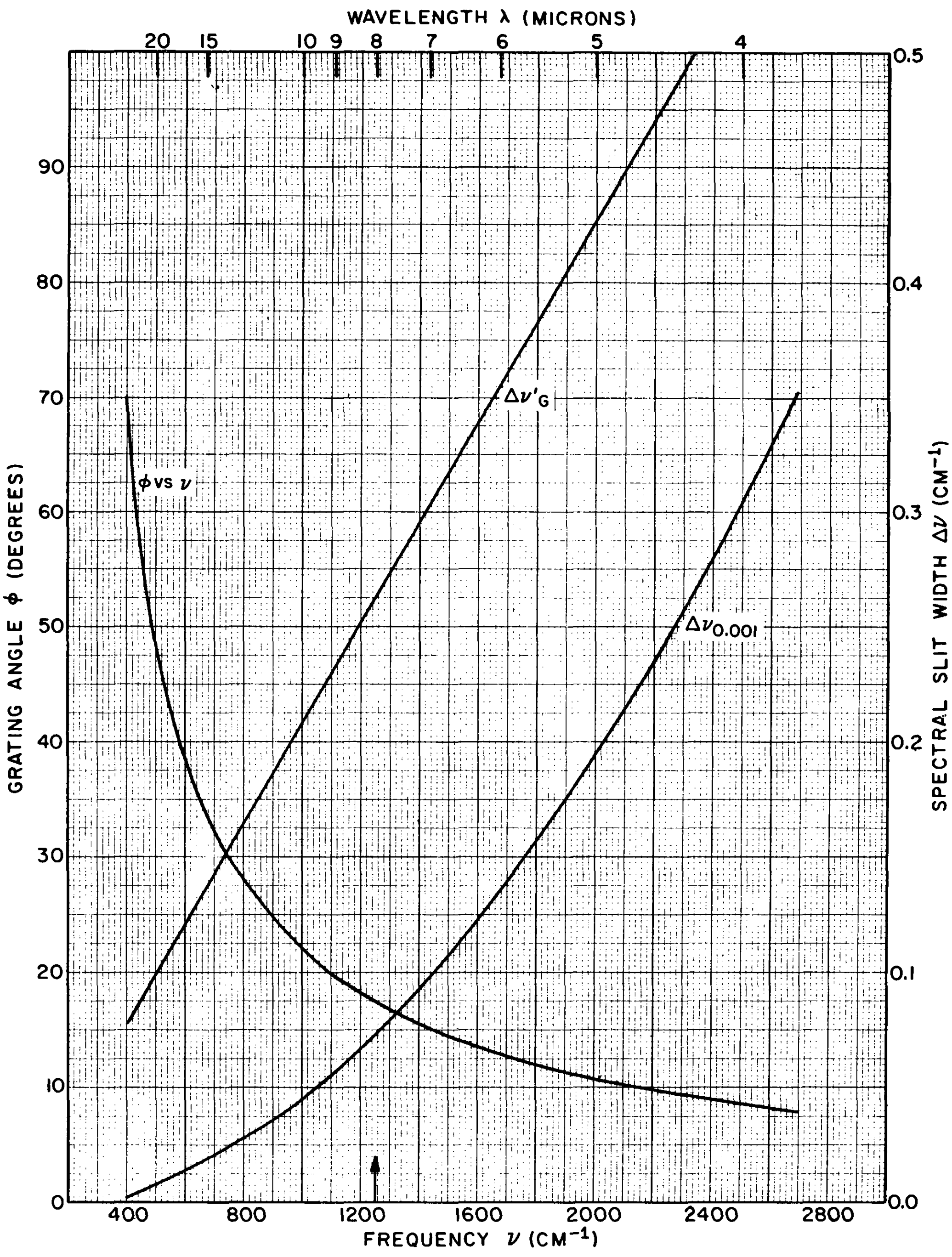

Fig. 28 - Resolution of a grating with a blaze wavelength = 8.0 μ, d = 1/750 = 1.33×10^{-3} cm, and R_0 = 4800

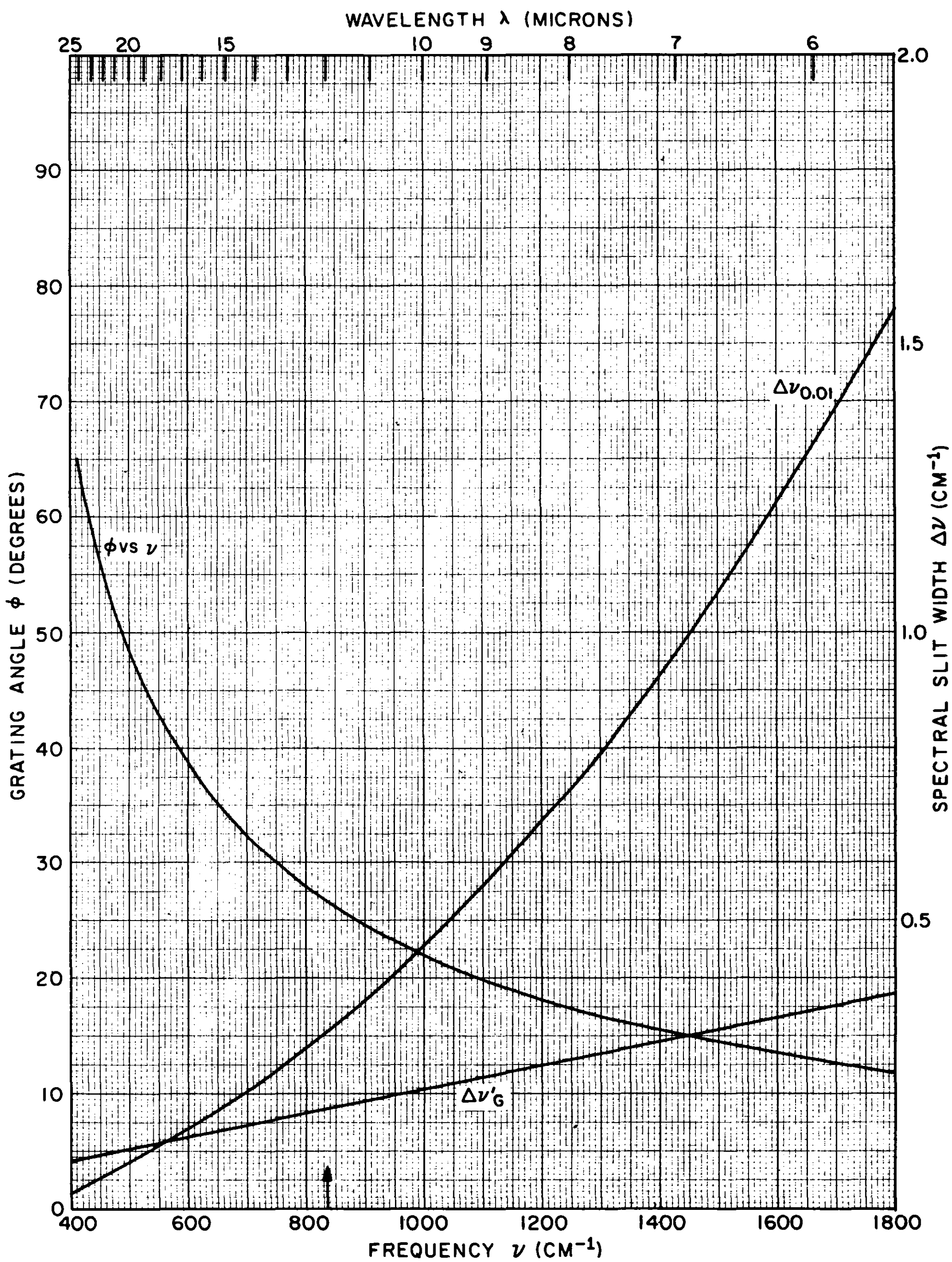

Fig. 29 - Resolution of a grating with a blaze wavelength = 12.0 μ, d = 1/750 = 1.33×10^{-3} cm, and R_0 = 4800

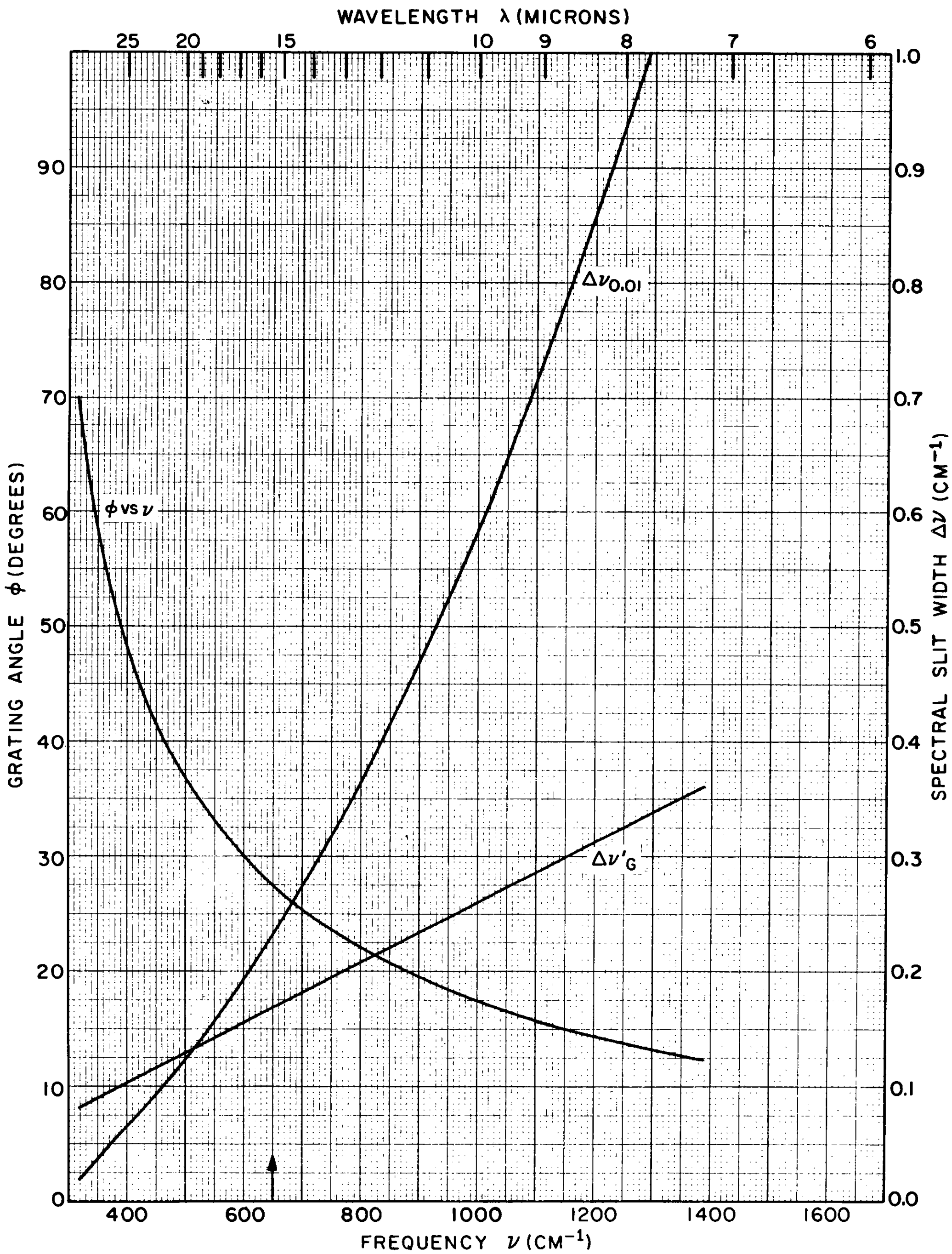

Fig. 30 - Resolution of a grating with a blaze wavelength = 16.0 μ, $d = 1/600 = 1.66 \times 10^{-3}$ cm, and $R_0 = 3840$

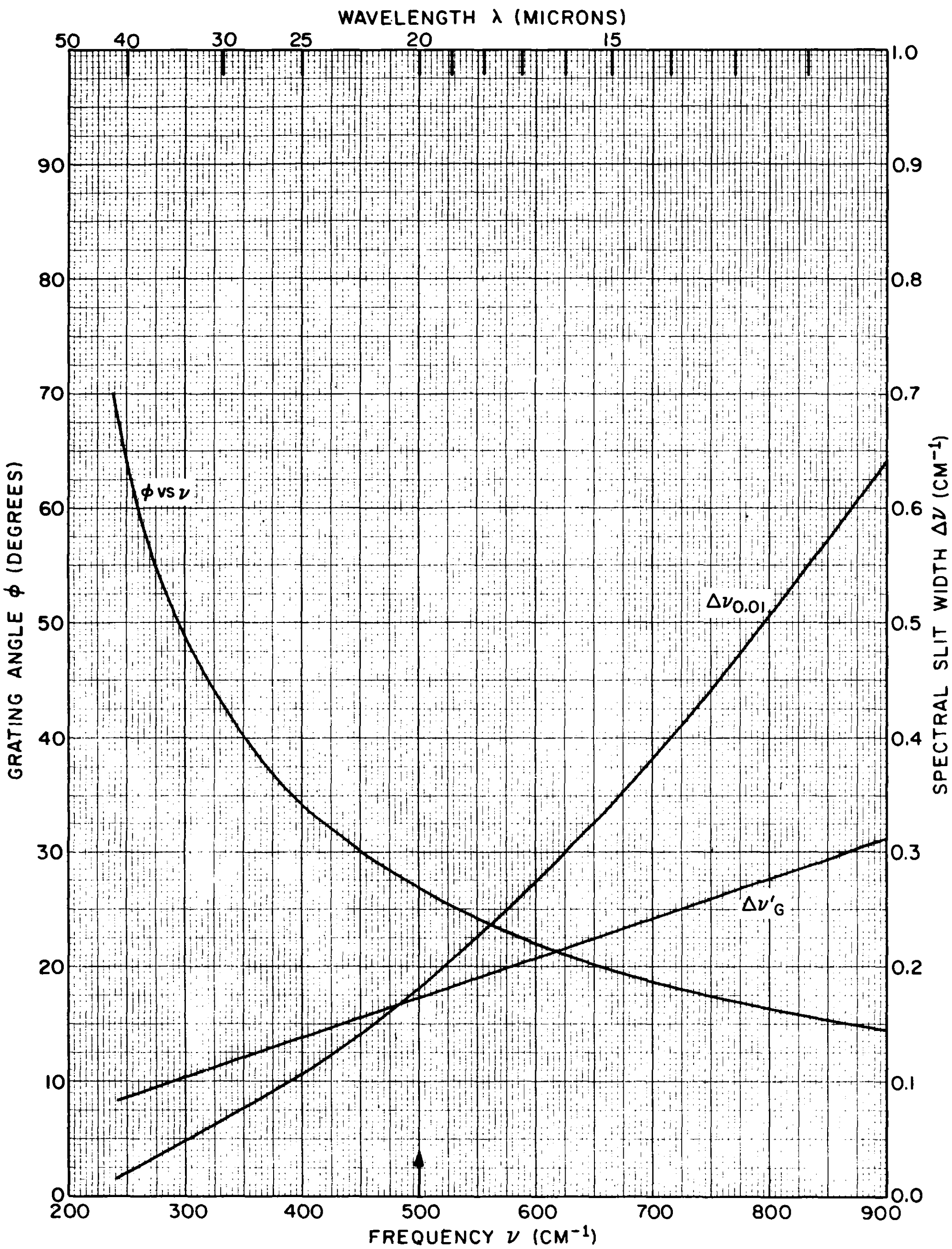

Fig. 31 - Resolution of a grating with a blaze wavelength = 20.0 μ, $d = 1/450 = 2.22 \times 10^{-3}$ cm, and $R_0 = 2880$

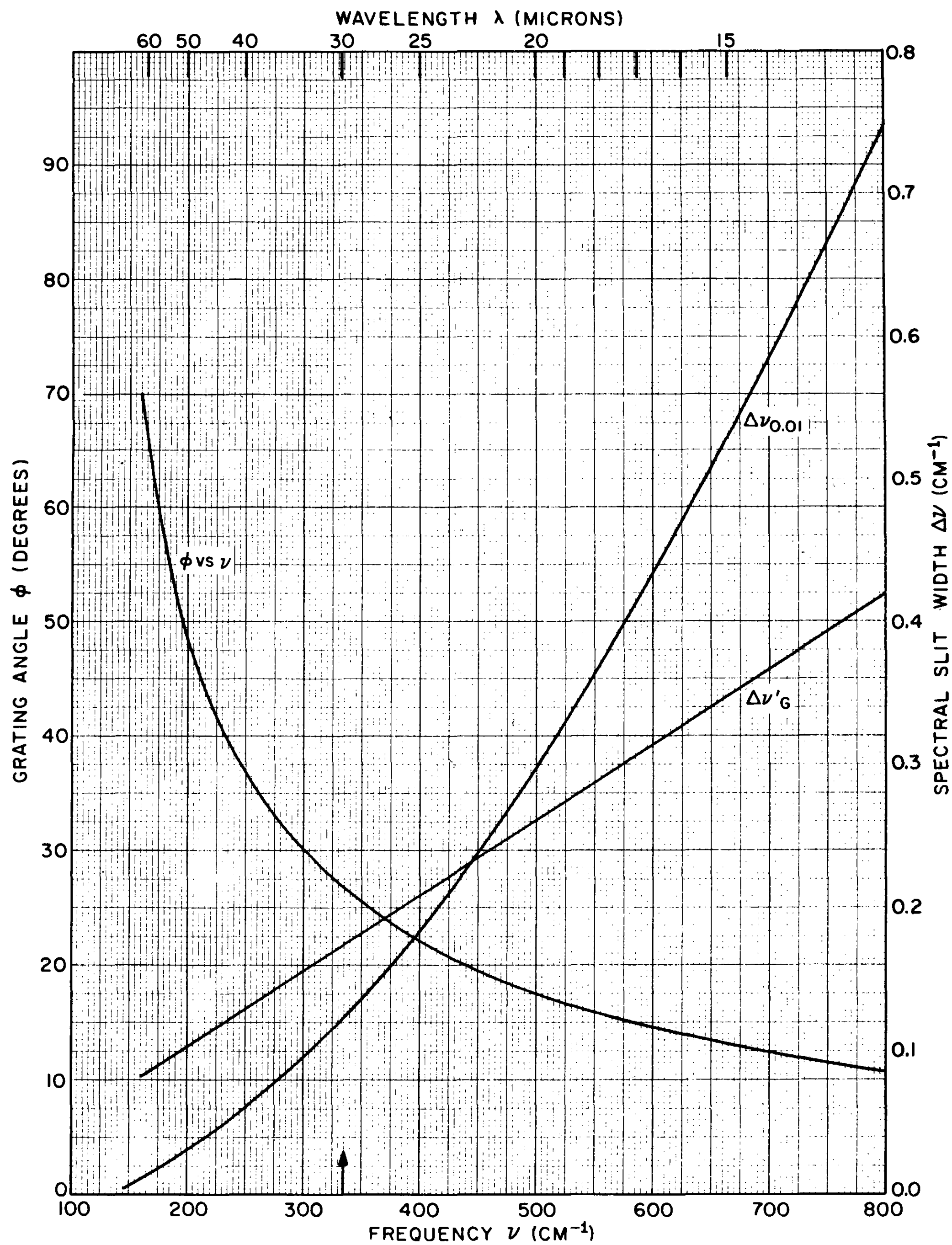

Fig. 32 - Resolution of a grating with a blaze wavelength = 30.0 μ, $d = 1/300 = 3.33 \times 10^{-3}$ cm, and $R_0 = 1920$

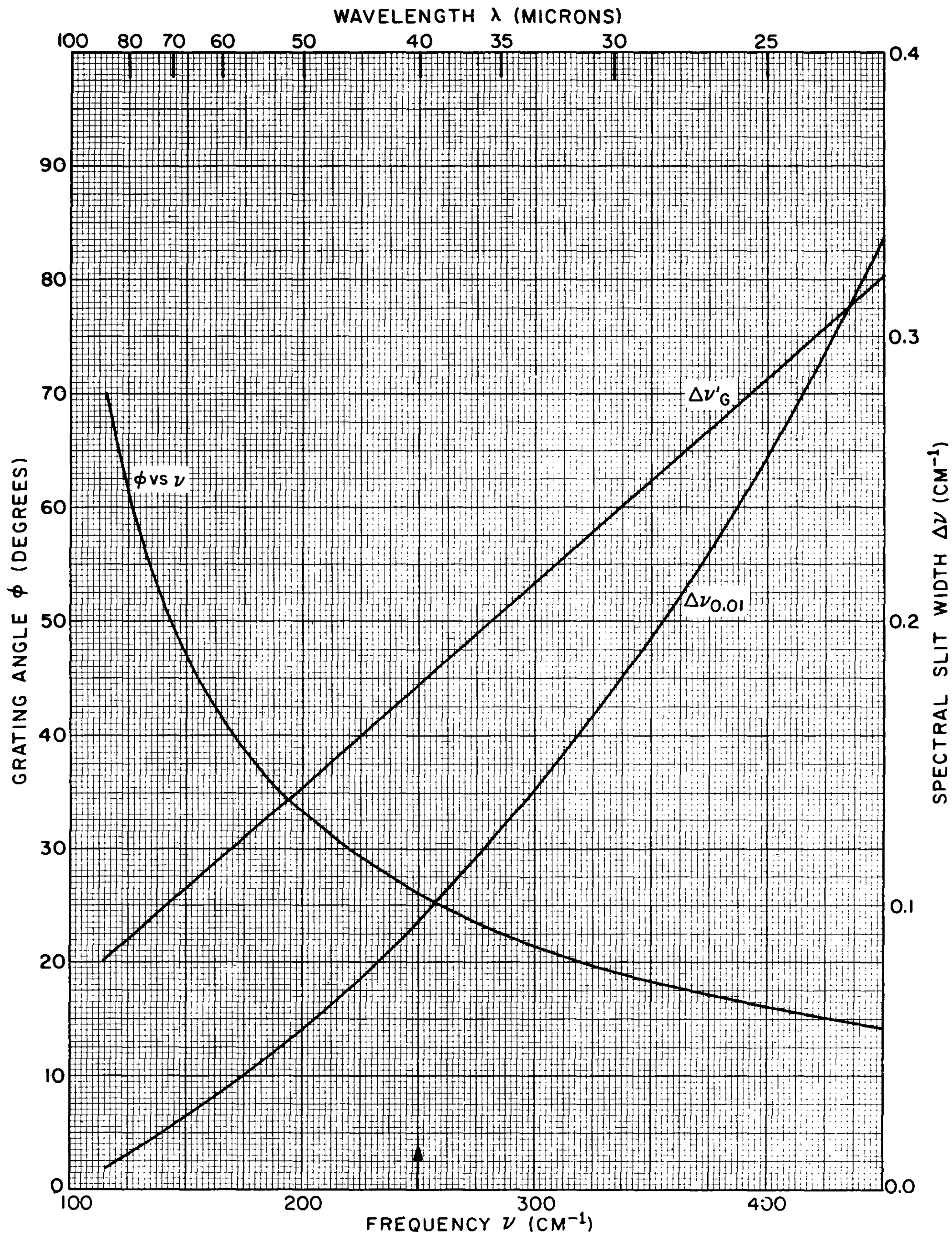

Fig. 33 - Resolution of a grating with a blaze wavelength = 40 μ, d = 1/219 = 4.57 × 10^{-3} cm, and R_0 = 1400

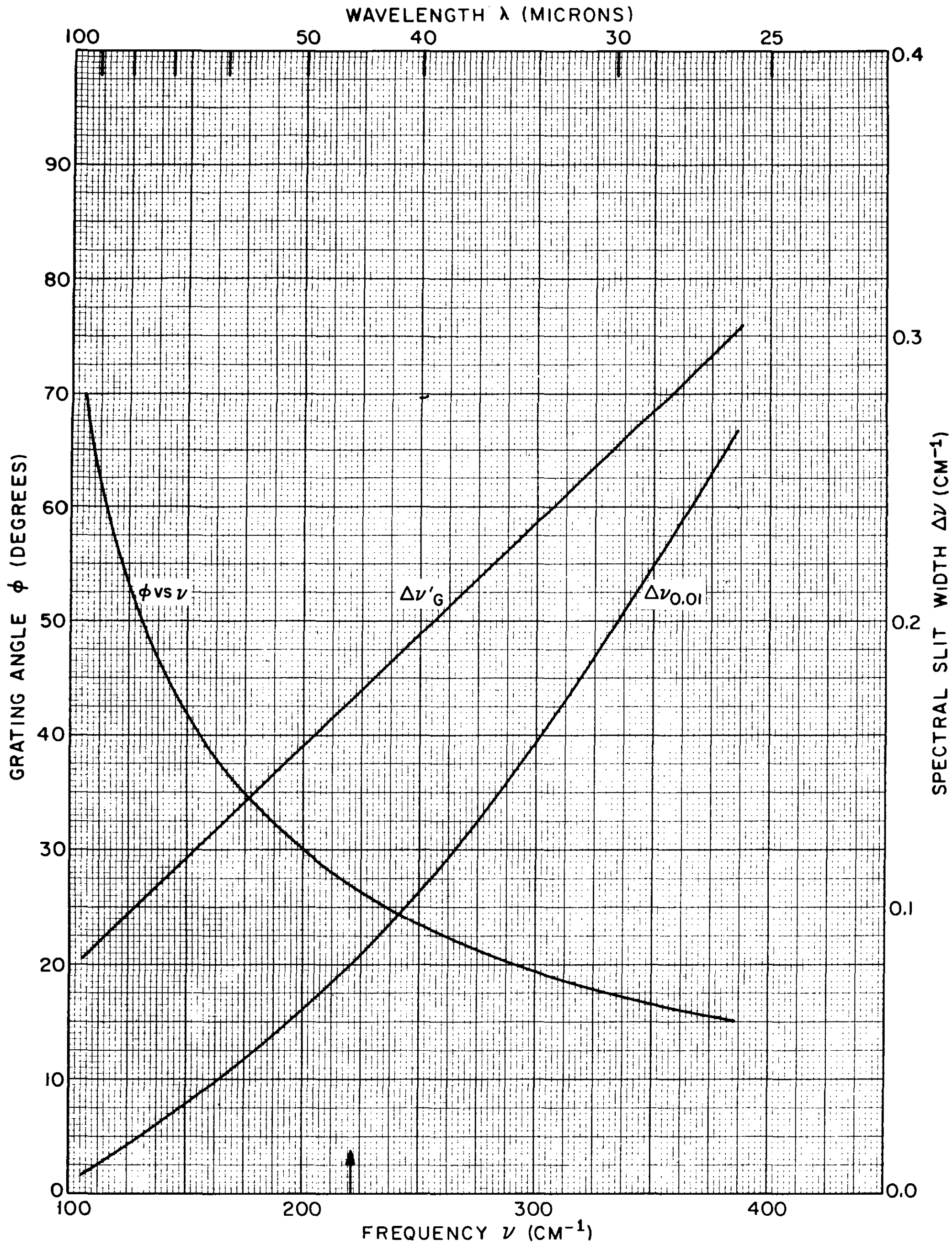

Fig. 34 - Resolution of a grating with a blaze wavelength = 45.0 μ, d = 1/200 = 5.0×10^{-3} cm, and R_0 = 1280

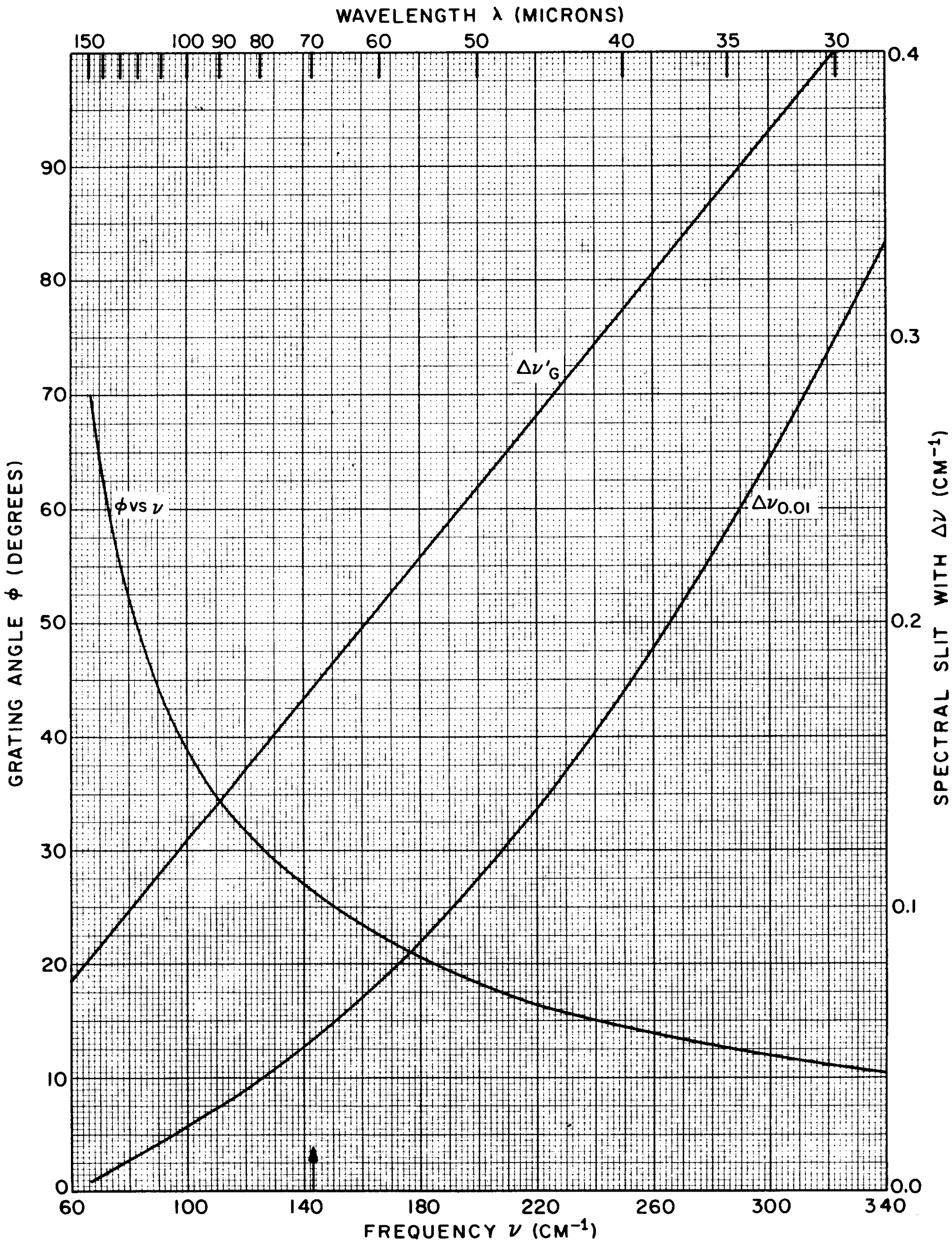

Fig. 35 - Resolution of a grating with a blaze wavelength = 70 μ, d = 1/126 = 7.94×10^{-3} cm, and R_0 = 806

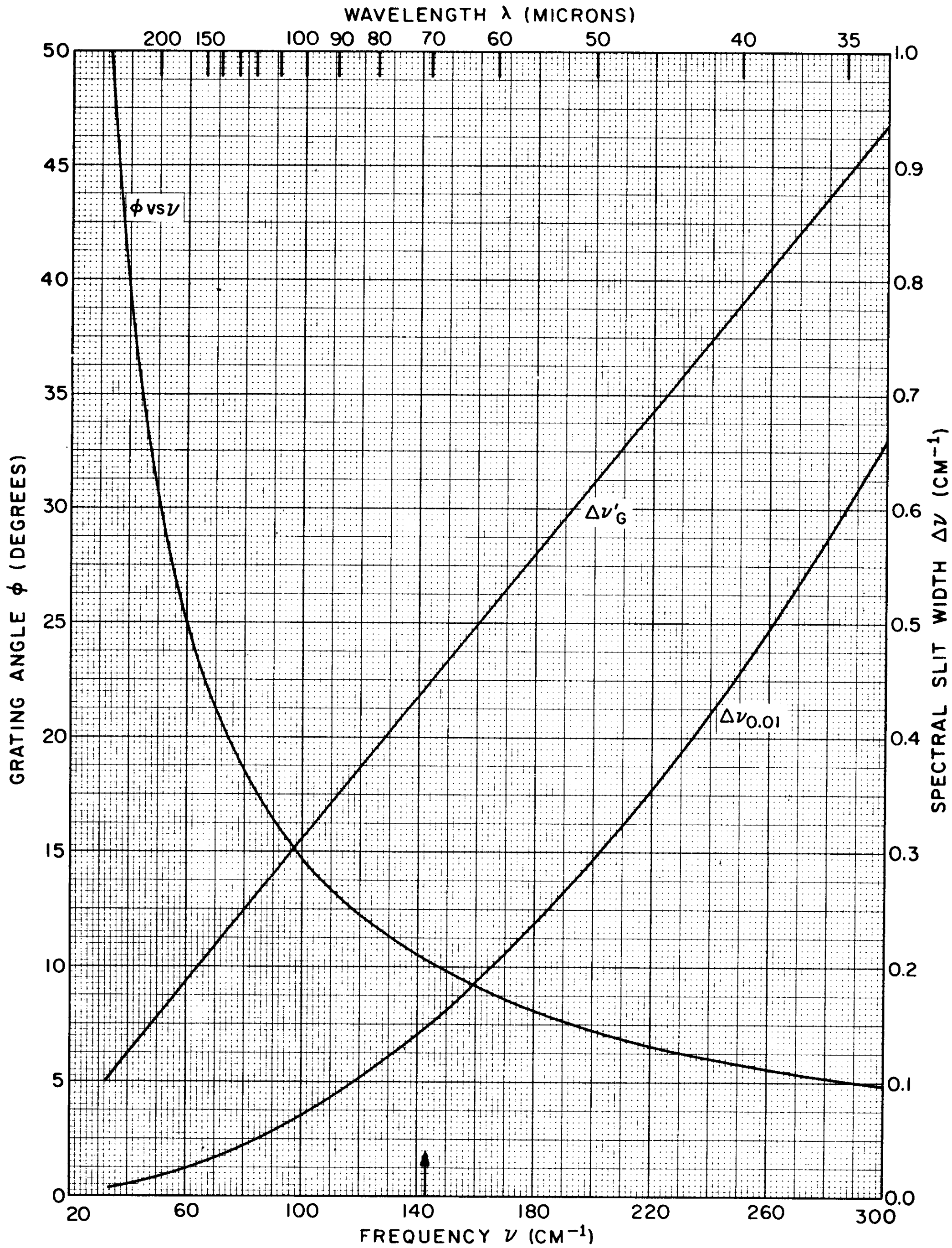

Fig. 36 - Resolution of a grating with a blaze wavelength = 70 μ, $d = 1/50.4 = 0.0199$ cm, and $R_0 = 322$

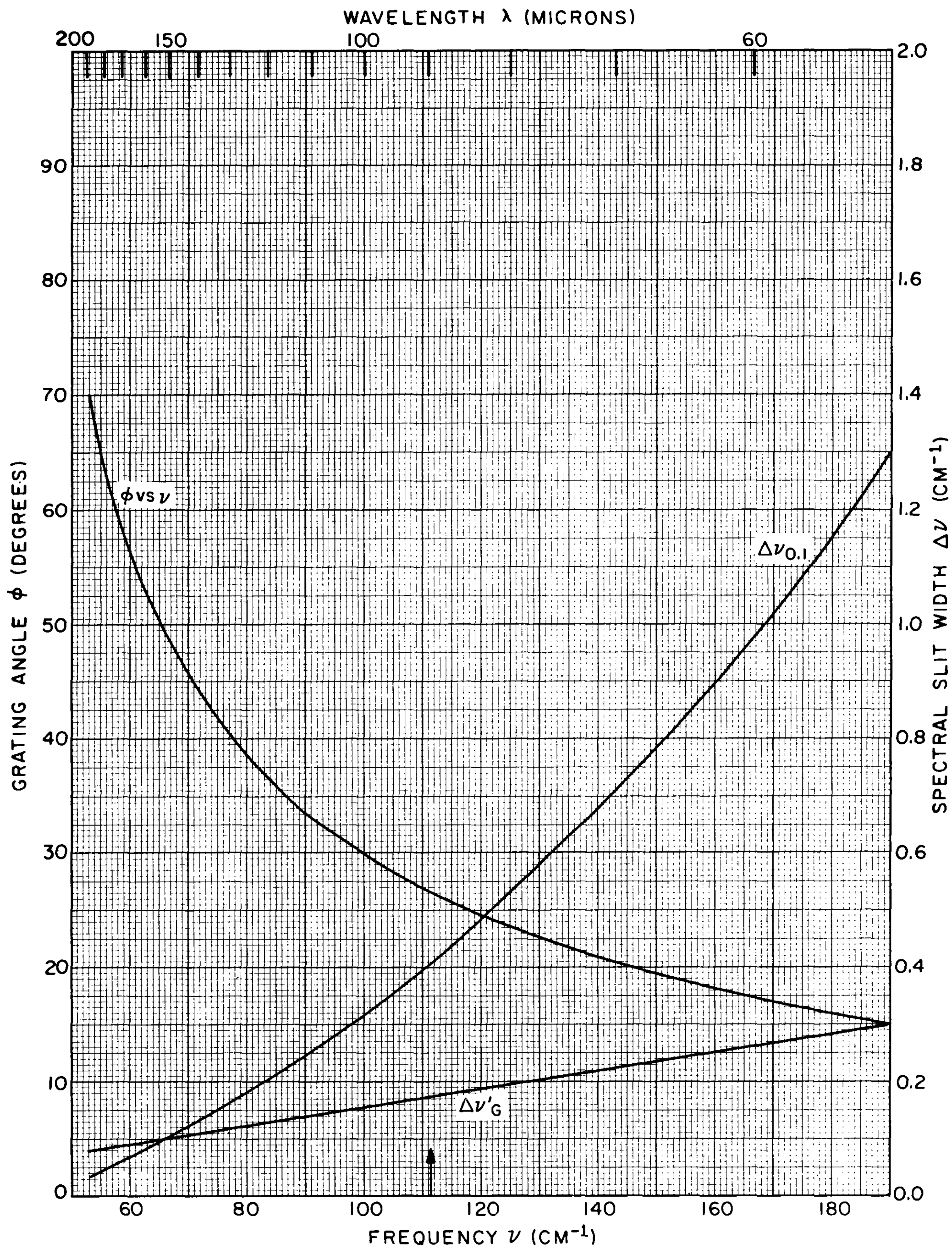

Fig. 37 - Resolution of a grating with a blaze wavelength = 90 μ, d = 1/100 = 0.01 cm, and R_0 = 640

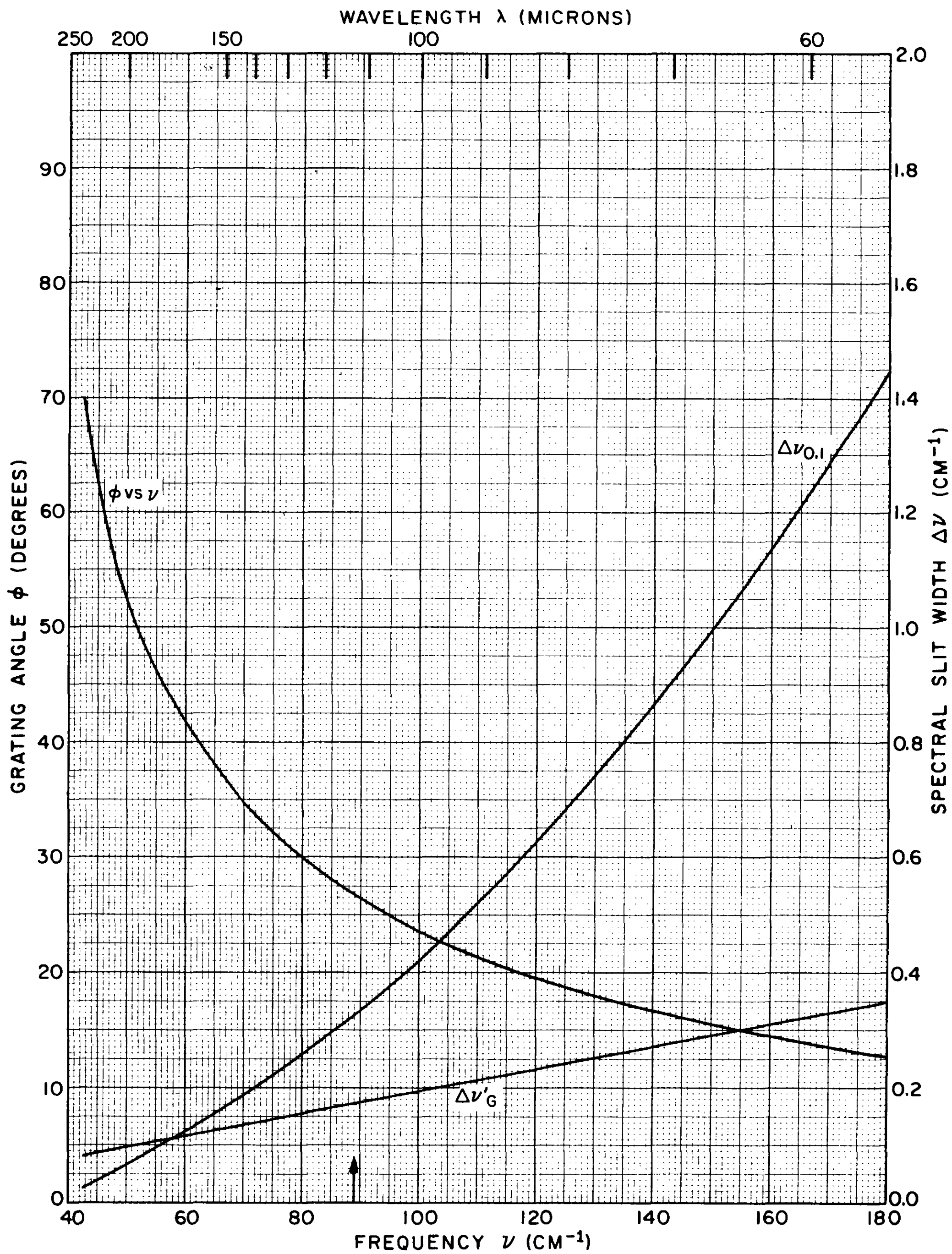

Fig. 38 - Resolution of a grating with a blaze wavelength = 112.5 μ, d = 1/80 = 0.0125 cm, and R_0 = 512

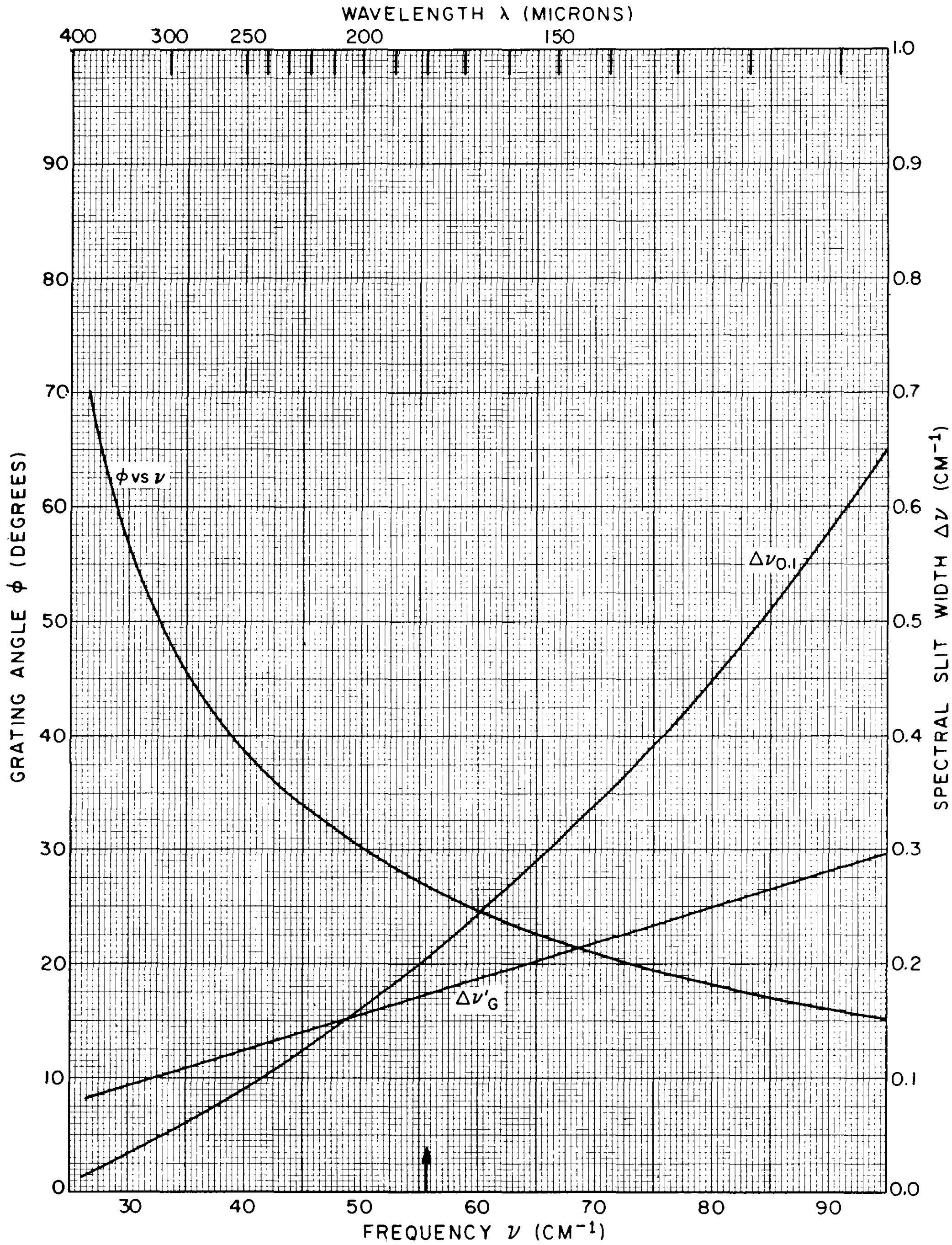

Fig. 39 - Resolution of a grating with a blaze wavelength = 180 μ, $d = 1/50 = 0.02$ cm, and $R_0 = 320$

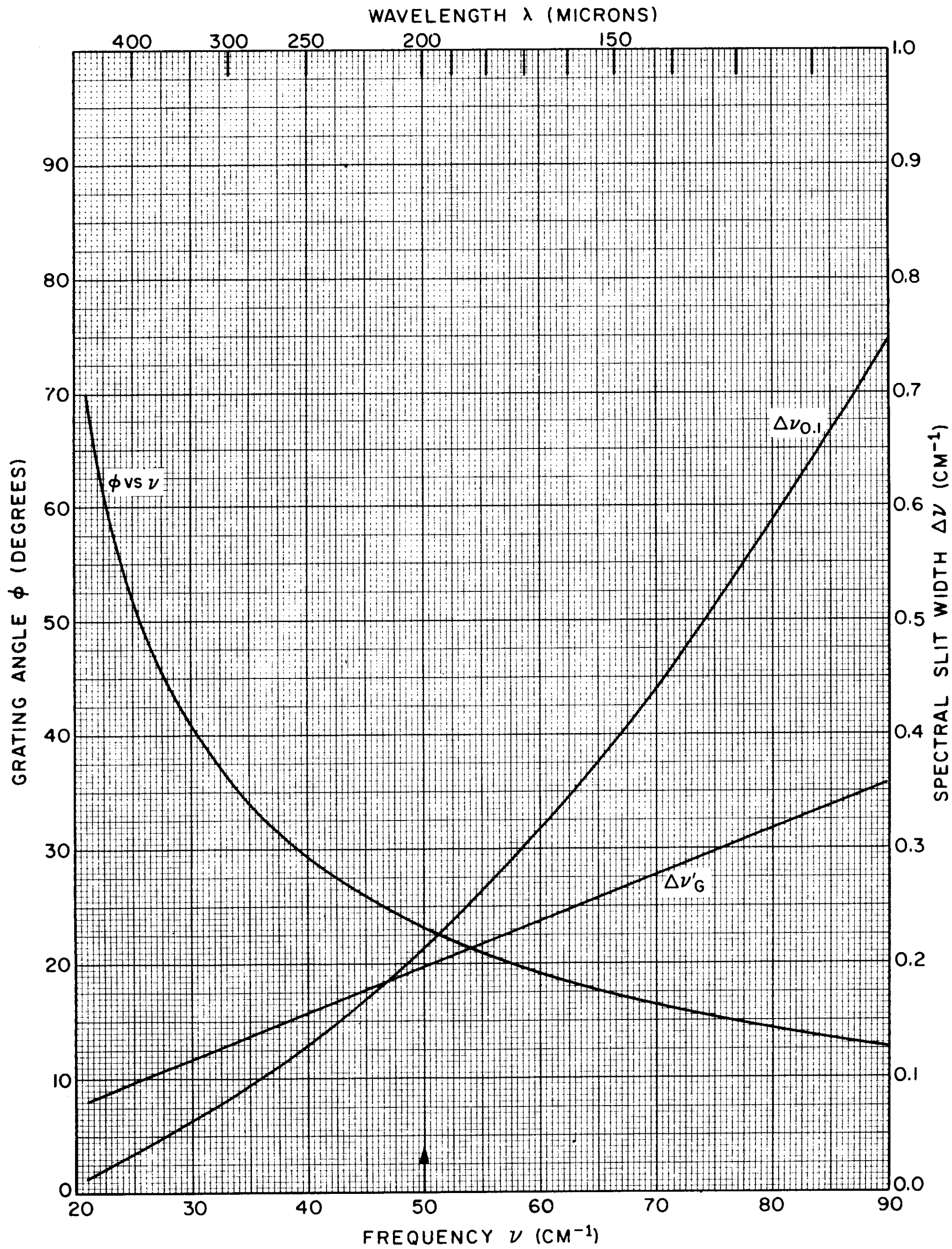

Fig. 40 - Resolution of a grating with a blaze wavelength = 200 μ, d = 1/39.4 = 0.0254 cm, and R_0 = 252

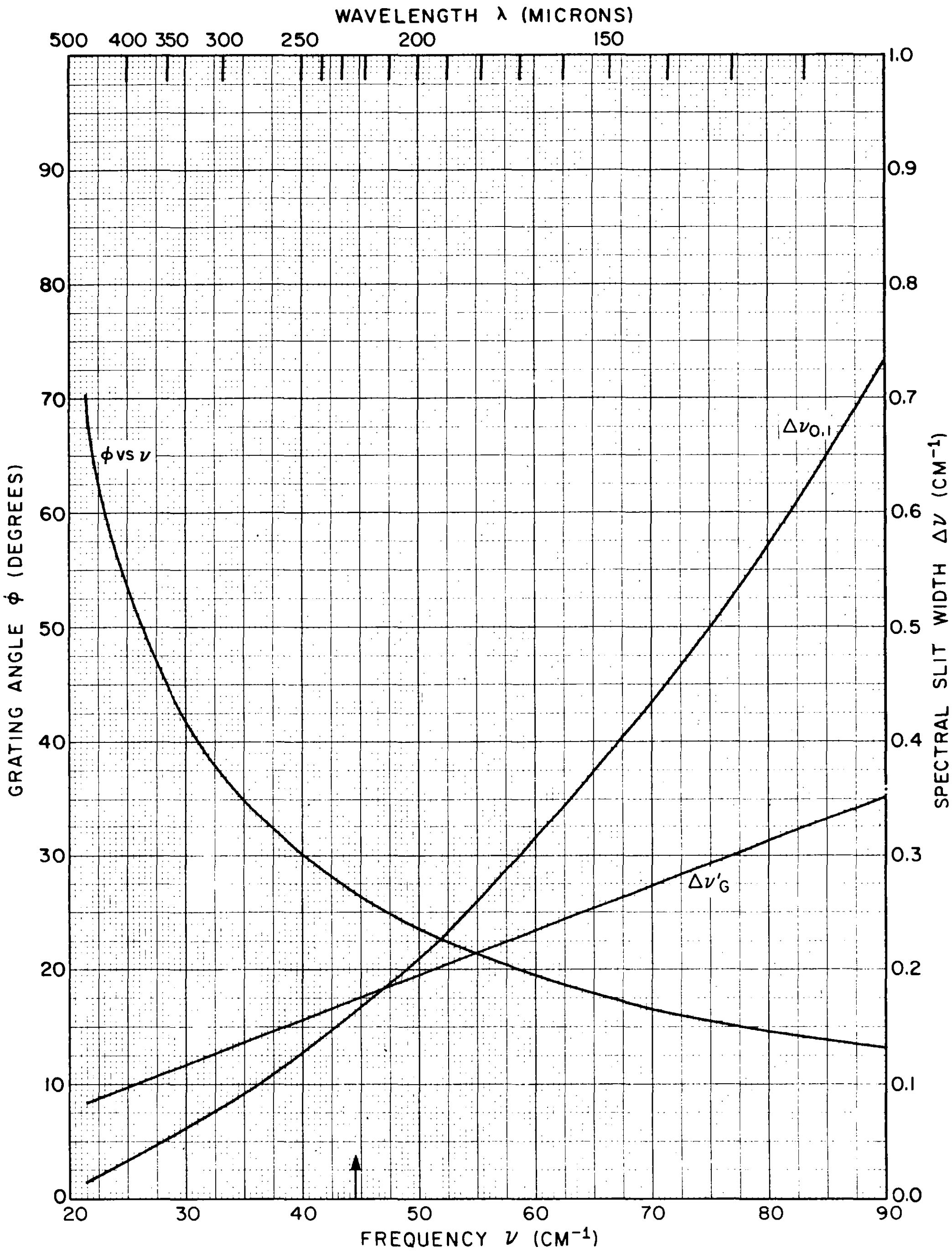

Fig. 41 - Resolution of a grating with a blaze wavelength = 225 μ, d = 1/40 = 0.025 cm, and R_0 = 256

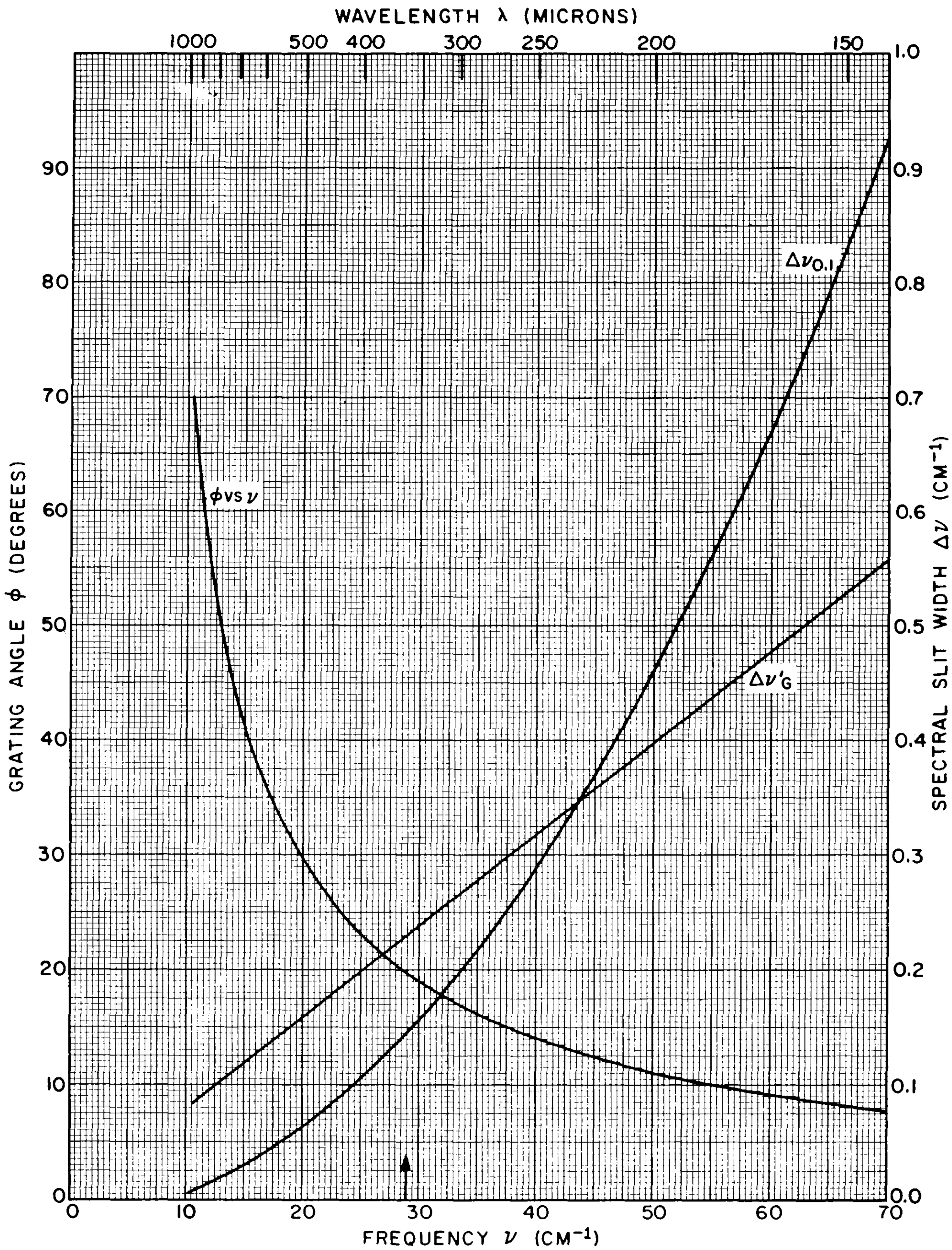

Fig. 42 - Resolution of a grating with a blaze wavelength = 347 μ, d = 1/19.7 = 0.0507 cm, and R_0 = 126

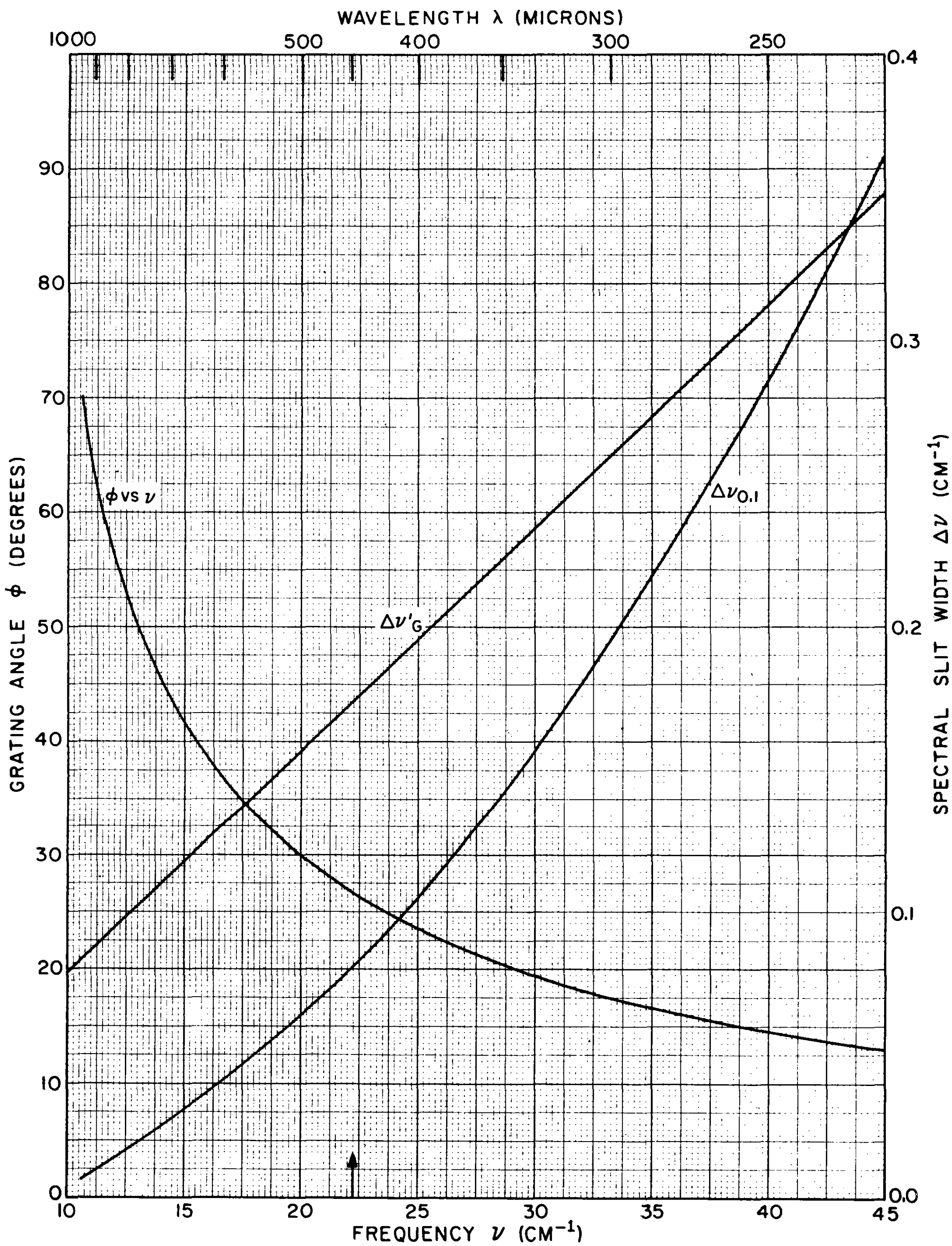

Fig. 43 - Resolution of a grating with a blaze wavelength = 450 μ, d = 1/20 = 0.05 cm, and R_0 = 128

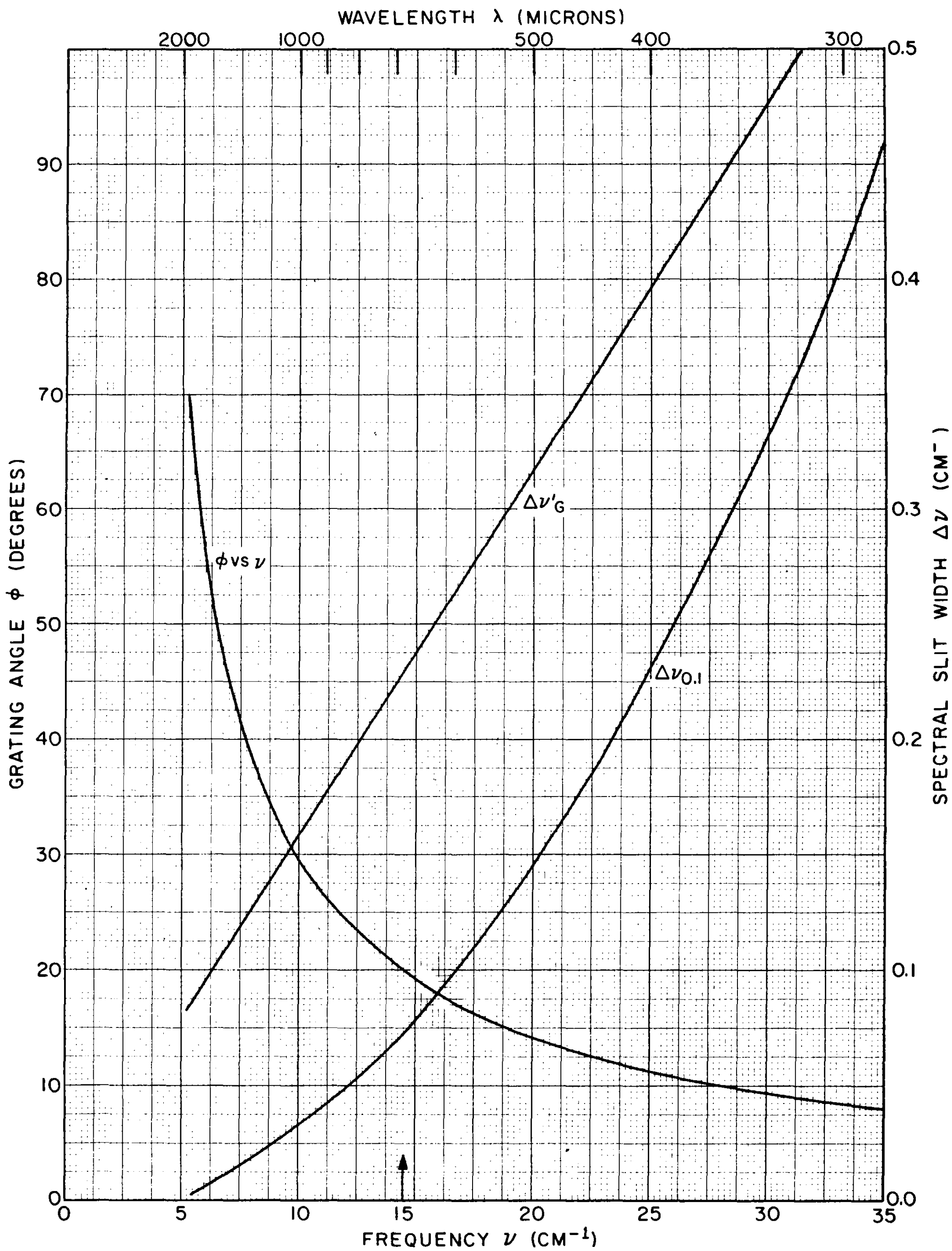

Fig. 44 - Resolution of a grating with a blaze wavelength = 694 μ, d = 1/9.85 = 0.1015 cm, and R_0 = 63

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DOCUMENT CONTROL DATA - R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

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13. ABSTRACT

A simple derivation of the spectral resolution of the standard Perkin-Elmer prism and grating monochromators (Models 12-C and 12-G) has been carried out. Some attention is given to discussion of the variation of the diffraction pattern width at the exit slit as a function of the physical width of the entrance slit. Brief mention of power considerations is also made. The resulting formulas have been used to calculate spectral slit width curves for eight different prisms and twenty-six gratings. The spectral slit width in cm^{-1} is plotted as a function of the frequency in cm^{-1} and wavelength in microns. These detailed graphs allow a determination of spectral slit width from quick inspection.

DD FORM 1 JAN 64 1473

Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Infrared spectroscopy Prism monochromator Grating monochromator Spectral resolution Mathematical derivation Calculations Spectral slit width curves Signal power						

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