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Modeling variation in the refractive index of optical glasses

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Modeling Variation in the Refractive Index of Optical Glasses

by

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A thesis submitted in partial fulfillment
of the requirements for the degree of
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Submitted to the
Center for Imaging Science
in partial fulfillment of the requirements
for the Master of Science Degree
at the Rochester Institute of Technology

Abstract

Experimental measurements that describe the dispersive behavior of production samples of optical glasses are fit with models of minimum complexity for the purpose of interpolation and extrapolation. Software to perform this procedure on a regular basis is presented, and shown to distinguish between models of inappropriate complexity. Two degrees of freedom usually provide a statistically optimum fit to the data—contrary to the widespread practice of fitting a general, six term model to such measurements.

Using specially developed analysis tools, it is concluded that annealing does not significantly change the partial dispersion of the sample. Partial dispersion is established at the time the ingredients are combined in a melt and is invariant from one annealing to another. This is an important result to consider when planning the fabrication of optical systems whose prescription changes with changes in material characteristics.

Acknowledgements

I wish to thank Mike Mandina, General Manager of Melles Griot (Optics Division), in Rochester NY, for sponsoring this research; Andrea Hopkins and Publish*Ease* for the production of the diagrams; Schott Optical Technologies and Ohara Corporation, Inc., for sample measurement assistance; Gaertner Scientific Corporation for their help in refurbishing the spectrometer, and for the photograph shown in Figure 5; and my Committee for their support over the years.

Dedication

For my brother Chris

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I. Introduction

• Description

As optical objectives become more complex with performance routinely expected at or near the diffraction limit, competition is forcing companies to reduce material costs, labor, and lead time required to manufacture them. The tolerance budget is directly affected. Few companies can afford to specify extraordinarily tight tolerances on optical components and subassemblies. While this practice will generally guarantee a high percentage of good assemblies, it also increases material cost, labor, and fabrication time to an unacceptable level.

The optical shop is most efficient when fabricating to *commercial* manufacturing tolerances. Commercial parts often have too much variability to guarantee that they will lead to diffraction-limited assemblies, however. Methods of compensating for the use of these parts must be implemented if attractive delivery time and price are to be attained. This compensation must take the form of adjustments to the optical and mechanical designs to allow the use of these commercial-grade components to create an objective that forms a perfect image. This analysis and adjustment must often be done on an assembly-by-assembly basis.

Optical components depart from their nominal characteristics in two ways. *Power* errors are those which result in rotationally symmetric image quality degradations. Element surface curvatures, thicknesses, separations, and refractive indices all cause varying degrees of symmetrical degradations since the power balance of the objective is upset by their departure from nominal. The power balance can often be restored by deliberately changing another source of power error to add an equal and opposite amount. The offending parameter often goes uncorrected, in the true sense.

Asymmetrical image quality degradations—those that are not rotationally symmetric about the optical axis—are the other symptom of optical component departures from nominal. Surface cylindrical irregularity, element wedge or decenter, and local refractive index gradients are but a partial list of potential sources. Most

often, performance is restored by correcting the offender, though compensating strategies are occasionally adopted.

This research has sought to characterize one cause of power errors: the departure of the bulk refractive index of the optical component from its nominal, expected value. When departures from nominal are small, compensation for the variation in raw material refractive index is accomplished by changing airspaces. For departures of greater magnitude, curve changes may be required. This adjustment, done prior to fabrication, is referred to as the *melt recomputation* and may result in a production nominal that is different from the design nominal. This is often repeated just prior to assembly when all other characteristics of the components are known.

The melt recomputation is complicated by the dispersive nature of optical glasses. Refractive index varies in a nonlinear fashion with wavelength. Figure 1 shows the dispersion function for two different optical glass types: SK-16 and F-2.

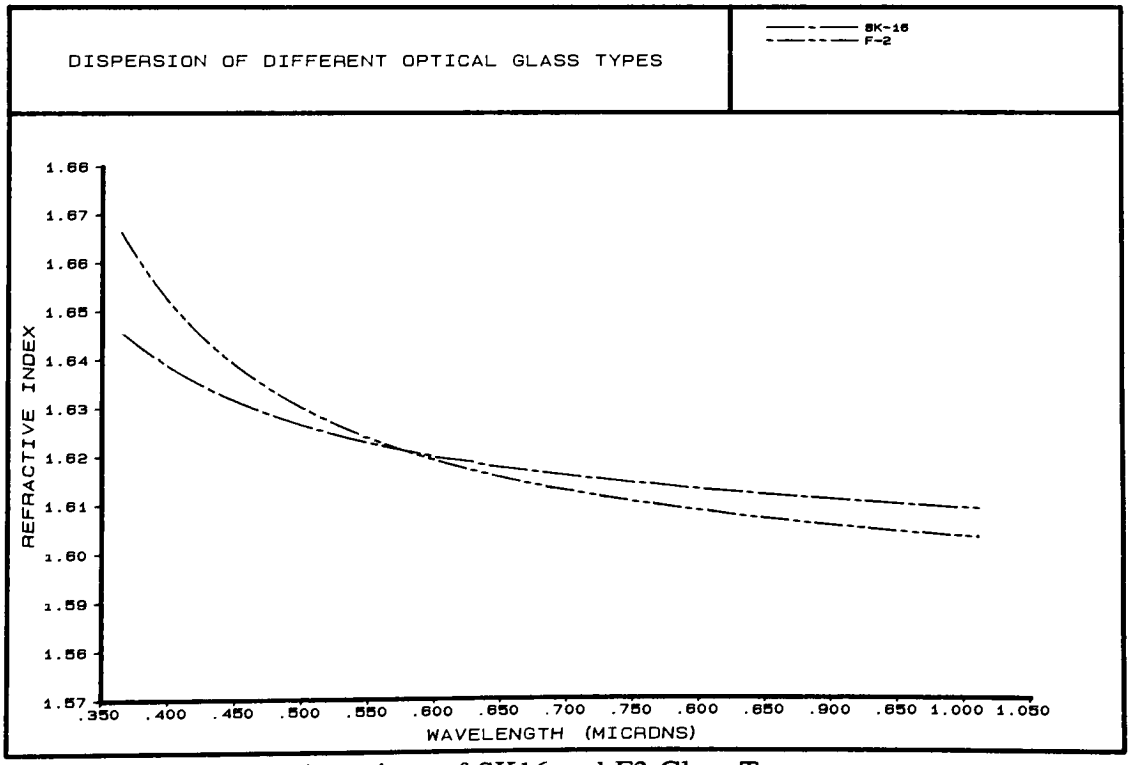

Figure 1 Different Dispersions of SK16 and F2 Glass Types

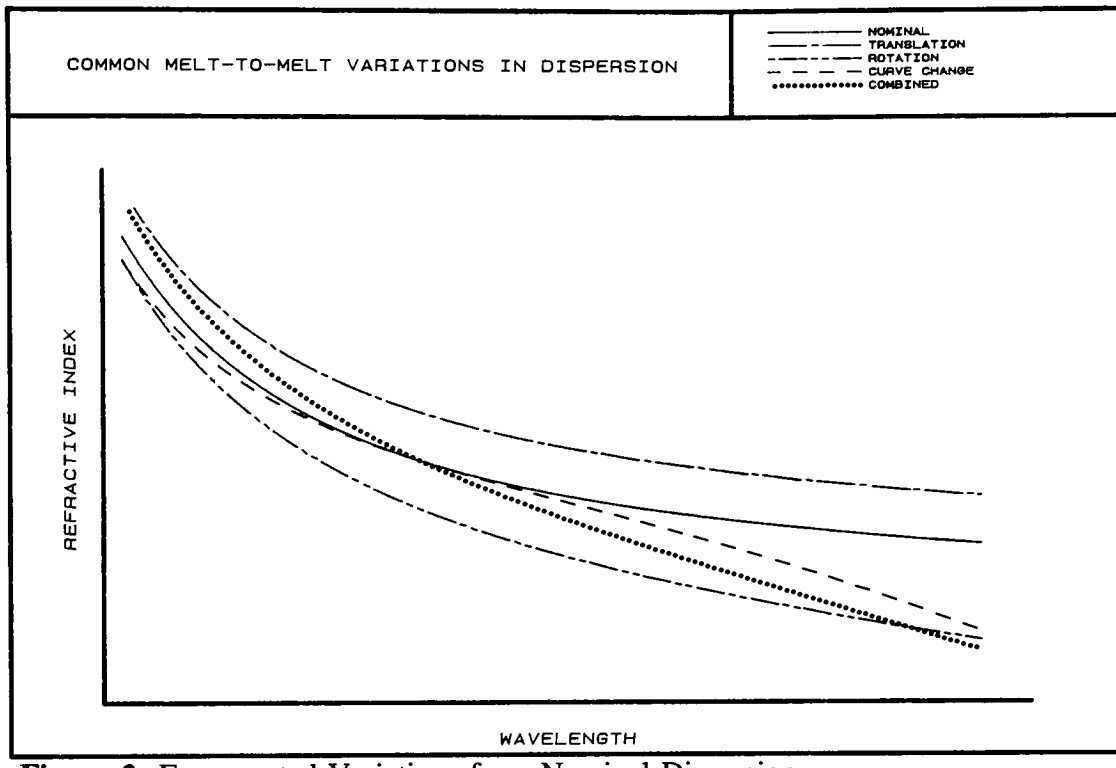

Figure 2 Exaggerated Variations from Nominal Dispersion

Figure 2 shows, in exaggerated scale, three common changes of $n(\lambda)$ from melt-to-melt and annealing-to-annealing for the same glass type. In practice, of course, all three changes occur simultaneously, but one is often the dominant effect. A shift or translation of the $n(\lambda)$ curve relative to nominal requires fewer compensating changes to the optical design than a change in the functional form or shape of $n(\lambda)$. Changes in the shape of $n(\lambda)$ almost always require element curvature changes; any technique used for the melt recomputation should alert the optical designer to changes in the shape of $n(\lambda)$ to allow a proper choice of variables and suggest possible performance problems.

The nominal dispersive behavior of optical glasses has been well catalogued by glass manufacturers.[1,2,3,4,5,6] The values reported are the result of experimental measurement of refractive index, n, at many wavelengths, λ, averaged over many melts. For objectives that are designed to operate over a range of wavelengths it is

necessary for the optical designer to determine what the actual dispersion $n(\lambda)$ is for every material in the optical path if maximum performance is to be attained.

It is often not possible to determine n at some λ of interest by direct experimentation due to the unavailability of suitable radiation sources. This implies that the melt recomputation method must be able to reliably interpolate over experimental data, smoothing experimental errors, and fitting with a nonlinear dispersion model. Minimizing the amount of experimental data required for reliable interpolation is an important goal since this problem is one encountered in a production situation, not an academic one.

• History

Modeling the dispersion of optical glass is a well studied topic. Most workers have concentrated either upon extracting maximum accuracy in index over the widest possible wavelength interval using the fewest possible coefficients, or upon developing a power series model for dispersion on which a theoretical model of the dispersive behavior of optical systems would be based.[7] Some have also investigated or proposed suitable models for dispersion in regions of the spectrum where the manufacturers do not supply data, namely the short ultraviolet (UV) region[8] and the long infrared (IR).[9]

In order to study the dispersive nature of optical systems using aberration coefficients it is necessary to express $n(\lambda)$ as a truncated power series. Standard methods of series manipulation cannot be utilized, nor is derivative manipulation feasible,[10] if another form is used. Buchdahl proposed a suitable equation[11] that was based on an analysis of the two-term Hartmann model,

$$n = n_0 + a\omega + b\omega^2 + c\omega^3 + \cdots, \qquad \omega = \frac{\lambda - \lambda_0}{1 + 2.5(\lambda - \lambda_0)} \quad . \tag{1}$$

Robb and Mercado recently analyzed the Buchdahl model, Eq. (1), and have found that, while it is not as accurate as the model adopted by the glass manufacturers, its accuracy is sufficient* to allow the theoretical modeling of the dispersive behavior of optical systems without producing misleading results[12].

The accuracy of alternative dispersion models is usually evaluated by comparing the index predicted by the model in question with the index predicted by the manufacturers' dispersion formula,[13]

$$n^2 = A_0 + A_1\lambda^2 + \frac{A_2}{\lambda^2} + \frac{A_3}{\lambda^4} + \frac{A_4}{\lambda^6} + \frac{A_5}{\lambda^8} \quad . \tag{2}$$

This Laurent series, which can be derived from either the classical or quantum dispersion models,[14] is valid over the wavelength interval from 0.365 μm to 1.014 μm with an index accuracy of ± 0.000005. Over the restricted range of 0.400 μm to 0.750 μm, it is accurate to ± 0.000003. The six coefficients A_0, A_1, ..., A_5 are determined by a least squares fit to equation (2) of experimental data, averaged over many samples and melts. It represents the manufacturers' best estimate of the nominal dispersive characteristics of the glass type in question. A set of these six coefficients is supplied for each of the more than 800 optical glass types currently availiable.

The importance of using least squares methods to determine the coefficients from experimental data is often understated in the literature. Most model formulations are polynomials. Exact fitting of a polynomial through data points that have experimental error often introduces unsatisfactory oscillatory structure into the interpolant.[15]

When basing the coefficients on more experimental data points than there are coefficients, a set of simultaneous equations cannot be cast and solved; the least

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* Accuracy is reported as ± 0.000010 for the spectral region from 0.400 μm to 0.700 μm with the series carried to order 2, and ± 0.000020 for the spectral region 0.365 μm to 1.014 μm with the series carried to order 3.

squares procedure is the only practical method. With more data points than parameters, its use results in the interpolant passing near each of the experimental data points, but not necessarily passing through them, such that the sum of squared errors between the observed and expected values is minimized. Buchdahl originally determined the coefficients for Eq. (1) by solving simultaneous equations; Robb and Mercado have shown that by using least squares techniques it is possible to reduce the index error by a factor of five over the same interval.[16]

While the manufacturers' dispersion formula (2) is almost an order of magnitude more accurate than the Buchdahl model (1), this does not diminish the usefulness of the latter. Equation (1) is suitable for the academic study of optical system dispersion by *orders*, just as the other primary optical aberrations have been studied (e.g., third-order spherical aberration, etc.); Eq. (2) is not suitable for this type of study. But Eq. (2), and any other form that was derived from either the classical or quantum theories of dispersion, has greater accuracy due to its physical basis. It is intended to be used when designing and manufacturing an objective. Both approaches are accurate enough for their intended applications.

Many other functional forms that have been proposed for dispersion modeling have been summarized in the literature. Some are empirical while others are based on the physical and chemical phenomena that give rise to the dispersive nature of optical glasses. A short list follows:

Cauchy[17]

$$n = A_0 + \frac{A_1}{\lambda^2} + \frac{A_2}{\lambda^4} \tag{3}$$

Conrady[18]

$$n = A_0 + \frac{A_1}{\lambda} + \frac{A_2}{\lambda^{3.5}} \tag{4}$$

Hartmann 1-term[19]

$$n = \frac{A_0}{(\lambda - \lambda_0)^{1.2}} \tag{5}$$

Hartmann 2-term[20]

$$n = A_0 + \frac{A_1}{(\lambda - \lambda_1)^{1.2}} \tag{6}$$

Hartmann 3-term[21]

$$n = A_0 + \frac{A_1}{(\lambda - \lambda_1)} + \frac{A_2}{(\lambda - \lambda_2)} \tag{7}$$

Lorentz-Lorenz[22]

$$\frac{n^2 - 1}{n^2 + 2} = \frac{N_0 e^2}{3\pi m} + \frac{A_1}{\upsilon_1^2 - \upsilon^2} + \cdots + \frac{A_j}{\upsilon_j^2 - \upsilon^2} + \cdots \tag{8}$$

Helmholtz[23]

$$n^2(1 - \kappa^2) = 1 + \frac{A_1\lambda^2}{\lambda^2 - \lambda_1^2 + \dfrac{g_1\lambda^2}{\lambda^2 - \lambda_1^2}} + \cdots + \frac{A_j\lambda^2}{\lambda^2 - \lambda_j^2 + \dfrac{g_j\lambda^2}{\lambda^2 - \lambda_j^2}} + \cdots \tag{9}$$

Sellmeier[24]

$$n^2 = 1 + \frac{A_1\lambda^2}{\lambda^2 - \lambda_1^2} + \cdots + \frac{A_j\lambda^2}{\lambda^2 - \lambda_j^2} + \cdots \tag{10}$$

Kettler-Drude[25,26]

$$n^2 = A_0 + \frac{A_1}{\lambda^2 - \lambda_1^2} + \cdots + \frac{A_j}{\lambda^2 - \lambda_j^2} + \cdots \tag{11}$$

binomial[27]

$$n^2 = \cdots + A_{-1}\lambda^2 + A_0 + A_1\lambda^{-2} + A_2\lambda^{-4} + \cdots + A_j\lambda^{-2j} + \cdots \tag{12}$$

Herzberger (visible)[28]

$$n = AL^2 + BL + C + D\lambda^2, \qquad L = \frac{1}{\lambda^2 - \lambda_0^2}, \qquad \lambda_0 = 0.168\,\mu\text{m} \tag{13}$$

Herzberger (infrared)[29]

$$n = AL^2 + BL + C + D\lambda^2 + E\lambda^4, \qquad L = \frac{1}{\lambda^2 - \lambda_0^2}, \qquad \lambda_0 = 0.168\,\mu\text{m} \tag{14}$$

The empirical equations, Eqs. (3) through (7), are surprisingly accurate over the visible spectrum. All provide for one or more *absorption bands* by making index approach infinity* at particular wavelengths, λ_j, where the glass molecules resonate. They differ in the location of these wavelengths and in how many absorption bands are provided.[30,31]

The Cauchy and Conrady forms provide for only one absorption band located at a wavelength of zero. It can be shown that the index of refraction at a wavelength of zero is unity,[32] however, so one should not have high expectations for the performance of such models. Absorption bands are known to exist on both sides of the visible region, one in the near UV and another in the far IR.[33] The Hartmann formulas, Eqs. (5) through (7), provide for one or more such absorption bands at nonzero wavelengths and, consequently, are of improved accuracy.

The Hartmann models may, at first, seem especially well suited for situations where little experimental information is available regarding the actual dispersion of a

* Algebraically, these singularities are caused by formulating the model so that the denominator of one or more terms goes to zero at λ_j, making index approach infinity. In actuality, of course, index does not become infinite at these wavelengths; it is only anomalies in the dispersion curve that occur. But since little use of the optical material is made at or near these absorption bands, the infinite index artifact of the algebraic formulation does not diminish the usefulness of the models.

sample. Instead of determining the absorption wavelengths with the other coefficients by solving simultaneous equations or by least squares, they may simply be assigned values that are realistic though, perhaps, not optimum. This reduces the number of coefficients that must be determined from the scarce experimental data.

For example, if for Eq. (5) we assume $\lambda_0 = 0.168$ μm, which is the mean absorption band central wavelength reported by Herzberger,[34] it can be rewritten as*

$$A_0 = n(\lambda - 0.168\,\mu\text{m}) \quad . \tag{15}$$

Upon substituting one experimentally determined wavelength and index pair, say λ_d and n_d, the coefficient A_0 is found. A rough estimate of index at some other wavelength may then be performed.

As might be expected, such a simple-minded approach is of low reliability. Suppose, for example, that two different glass types, each with the same n_d but different reciprocal relative dispersions, V_d, are compared with this approach. The interpolated indices will be equal. Yet, as shown in Figure 1, their dispersions may be very different.

Dispersion is reportedly determined by the chemical composition of the glass at the time of the melt.[35] During annealing, stress is relieved, homogeneity is improved, and index is adjusted to within a specified tolerance from nominal at one wavelength (usually λ_d). But the effect of annealing on the reciprocal relative dispersion, the so called *Abbe number*,

* In the course of performing this research, it has been found that much better results are obtained if the quantity (λ-0.168μm) is raised to the 0.012 power rather than the 1.2 power when the wavelength units are microns. This is true even if the 0.168 μm value is subsequently allowed to vary during optimization of Eq. (5) to experimental data. Equation (6) benefits from the same modification.

$$V_d = \frac{n_d - 1}{n_F - n_C} \quad , \tag{16}$$

is minor. The quantity n_d-1 changes with annealing, but the *principal dispersion*, the quantity n_F-n_C, does not [see Appendix 1, page 74]. While there are any number of combinations of n_F and n_C that could occur and keep the principal dispersion invariant with annealing, with only a single experimental data point the optical designer must assume that n_F, n_C, and n_d have all changed by the same amount. The result is that the actual $n(\lambda)$ curve is parallel to the nominal $n_0(\lambda)$ curve, as shown by the translation case in Figure 2.*

An improvement in the interpolation accuracy over that provided by empirical equations occurs when chemical and physical theory is used to suggest a dispersion model. With the Lorentz-Lorenz series, Eq. (8), index is, in general, complex-valued** although only the real terms are shown here.[36] The imaginary component becomes significant in the region of an absorption band and may, for most practical situations in the design and fabrication of optical objectives, be ignored. Note that Eq. (8) is a function of frequency instead of wavelength, where $\upsilon = c/\lambda$ and $c = 3 \times 10^8$ m/s. The Lorentz-Lorenz equation is the fundamental equation of classical dispersion theory;[37] e is the charge of an electron, m is the mass of an electron, N_0 is Avogadro's number, and the quantity A_j is related to the strength of the absorption that occurs at and about the frequency υ_j. One term is carried for each of the absorption bands characteristic of the material. This equation may be simplified when not used

* The experimental portion of this research will test this conclusion, which is based on the simple analysis presented in Appendix 1, by determining whether samples (which are all from the same melt but different annealings), all have $n(\lambda)$ curves which are parallel to one another within experimental accuracy.

** Ditchburn describes why the index must be complex in order to build a relationship that defines the polarization vector of the wave in the dielectric (glass) as a function of the incident electric field vector.

to model dispersion near these absorption bands. The Sellmeier series, Eq. (10), results.[38,39]

The Helmholtz series, Eq. (9), gives the real component of index as a function of wavelength with or without absorption bands in its range. It, too, has one term for each of the absorption bands that are characteristic of the material. The A_j coefficients have the same interpretation as when using the Lorentz-Lorenz equation. Used in ranges far from any absorption bands, the extinction coefficient, κ, and the terms multiplied by the damping coefficients, g_j, of the atomic oscillators become negligibly small reducing this equation, also, to the Sellmeier series, Eq. (10).[40]

The Sellmeier series is the most frequently used formulation for dispersion modeling. It is a valid approximation of both the classical Lorentz-Lorenz and Helmholtz equations when the range is not in the neighborhood of an absorption band.[41] For the visible spectral range, this includes all materials that are visually transparent. In the classical sense, the same number of terms are carried and the same interpretation is given to the A_j coefficients. When quantum mechanics is used as the theoretical basis, Eqs. (8) through (10) are still valid, but the number of oscillators (and thus the number of terms) is found to be infinite, and the A_j coefficients must be given a different interpretation.[42]

Fortunately, acceptable accuracy in the interpolated index can usually be obtained even when truncating the series after a reasonable number of terms,

$$n^2 = 1 + \frac{A_1\lambda^2}{\lambda^2 - \lambda_1^2} + \frac{A_2\lambda^2}{\lambda^2 - \lambda_2^2} + \frac{A_3\lambda^2}{\lambda^2 - \lambda_3^2} \quad . \tag{17}$$

The same physical interpretation of λ_j and A_j should not be extended to a truncated Sellmeier series. While a 3-term formulation, Eq. (17), will often be more than adequate as an interpolant following a least squares determination of A_1, A_2, A_3, λ_1, λ_2, and λ_3, one should not assume that absorption maxima occur at these three λ_j, nor

assume that the strengths of these absorption bands are proportional to the A_j coefficients.[43] All terms of the series are required for this interpretation. Also, it is important to remember that none of the absorption bands may occur within or near the range over which the Sellmeier series is defined for it to be valid.

It follows that the least squares solution for the truncated series, Eq. (17), will be better if the λ_j parameters are determined rather than assigned values based on experimental absorption data. This means that less precision will generally result if an attempt is made to reduce the amount of experimental data required by assigning known values to λ_1, λ_2, and λ_3 followed by the determination of A_1, A_2, and A_3 by linear least squares. This is unfortunate because Eq. (10), and truncated forms such as Eq. (17), are awkward to solve with least squares due to their nonlinearity. The Sellmeier forms can be linearized by clearing fractions so that standard linear least squares may be used.[44] But this transformation causes unequal weighting to be applied to data of various values of λ, which is difficult to defend. Least squares solutions to transformed equations do not necessarily constitute a best fit solution to the original untransformed case and should be avoided.

When the Kettler-Drude series, Eq. (11), is discussed in the literature it is always presented separately from the Sellmeier series, Eq. (10).[45,46] Appendix 2 [page 75] shows that the two series are equivalent. When Eq. (11) is expanded with the binomial theorem, Eq. (12) results.[47] Comparing Eqs. (2) and (12) reveals that Eq. (2) is a special truncated case of Eq. (12), with the coefficients of Eq. (2) renumbered to correspond to the manufacturers' usage.

The glass manufacturers have chosen this portion of the infinite series, Eq. (12), to represent index over the wavelength range from 0.365 μm to 1.014 μm with adequate accuracy. If more accuracy had been required in the ultraviolet than Eq. (2) provides, more low-order terms in λ would be included from Eq. (12) [i.e., λ^{-10}, λ^{-12}, etc.]. Similarly, if more accuracy were required in the infrared, more high-order terms would be included [i.e., λ^4, λ^6, etc.].

Herzberger has proposed Eqs. (13) and (14) to model dispersion in the visible and infrared regions of the spectrum, respectively. The forms of the equations are similar to truncated forms of the Sellmeier or Kettler-Drude equations,[48] but the Herzberger equations are linear in their coefficients.

Accuracy suffers from the necessary approximations that allow this simplification. Indeed, Eq. (13) is noted by its author[49] to be an approximation of the nonlinear form,

$$n = \frac{A_1}{\lambda^2 - \lambda_1^2} + \frac{A_2}{\lambda^2 - \lambda_2^2} \quad , \tag{18}$$

which is, itself, only an approximation of the Kettler-Drude series [note that Eq. (11) yields n^2, not n]. Herzberger later notes[50] that a 5-coefficient truncated Sellmeier series [e.g., Eq. (18) with a constant term added] provides a better fit over the entire wavelength range from 0.58 μm to 11.9 μm than a piece-wise interpolant involving three separate invocations of Eq. (14). Historically, computational ease appears to have been a constraint that lead to this development. This is of less importance currently.

In summary, equations (10), (11), and (12), each being based on the Lorentz-Lorenz and Helmholtz equations, exhibit the same asymptotic behavior at several wavelengths.* Equation (12) doesn't just have one absorption band at a wavelength of zero, as a casual inspection may suggest. Truncated versions of Eq. (12), such as Eq. (2), approximate this behavior. It may be seen, then, that the manufacturers choice of Eq. (2) has a good basis in theory and it may be expanded in range in either direction as the need arises.

Further, although the form of the Sellmeier series is attractive since the λ_j and A_j parameters have physical significance, this cannot be claimed for the truncated, often-used, two- or three-term Sellmeier equations. No less information is conveyed

* None may be used in the neighborhood of these absorption bands, however.

by the truncated binomial expansion, Eq. (2), about the properties of the dispersive material. It is also linear in its coefficients. With this in mind, there seems to be little incentive to use anything but the form used by the manufacturers, Eq. (2).

• Research

It is possible to increase the accuracy of a statement that is made about the accuracy of experimental data by the proper mathematical treatment of the data and proper experiment design.[51] The primary purpose of this research was the development of a procedure that would allow optical designers to estimate refractive indices of optical glasses to a much greater accuracy than previously attainable, thereby enhancing the usefulness of their scarce experimental data.

The current state-of-the-art in fitting a curve to experimentally determined index of refraction data involves the fitting of a general dispersion model. All coefficients of the model are allowed as degrees of freedom.

The situation is similar to the following. Suppose that an experiment is performed which tested some dependent variable y that was known to vary with some independent variable x in a linear fashion. It would be incorrect for the analyst to fit the resulting data to the general polynomial,

$$y = A_0 + A_1 x + A_2 x^2 + A_3 x^3 + \cdots \quad , \tag{19}$$

of which the linear model is a special case, with the expectation that the coefficients of the high-order terms would be zero if the data truly described a linear relationship. It is exactly this type of approach that is taken when fitting a general dispersion model to experimental refractive index data, however.

It was proposed[52] that the *nominal* dispersion curve, $n_0(\lambda)$, for the glass type under test should be fit to experimental data, not the general dispersion model. The curve should be allowed to translate or tilt without its shape changing. Thus, the

complicated, nonlinear shape of $n_0(\lambda)$ is both provided and maintained, which is intuitively appealing since annealing is only supposed to translate the $n_0(\lambda)$ curve in the direction of the ordinate. It is not supposed to change its shape. If the general dispersion model were fit to the data instead, it would be difficult to constrain the resulting curve shape to be the same as $n_0(\lambda)$.

Such a procedure has been committed to software and will be used to test the following null hypothesis H_0:

> *Annealing causes a simple translation of the nominal curve, $n_0(\lambda)$, in the direction of the ordinate, but does not significantly alter the shape of the curve that is characteristic of the material.*

Figure 3 Null Hypothesis, H_0

Specifically, if it can be shown that samples have significantly different curve shapes, even though they are known to be from the same melt (but different annealings), then H_0 must be rejected and the alternate hypothesis H_1 accepted:

> *Annealing may significantly change the shape of the dispersion curve, $n(\lambda)$, so that a simple translation of the nominal curve, $n_0(\lambda)$, in the direction of the ordinate does not adequately explain the observed variation.*

Figure 4 Alternate Hypothesis, H_1

The procedure allows more complicated departures of $n(\lambda)$ from $n_0(\lambda)$ than a simple translation, but it is important to know when a simple translation is inadequate. When $n(\lambda)$ is allowed to change shape it may be necessary to alter the radius of curvature on one or more optical elements in the objective to compensate. Simple translations can usually be accommodated with simple airspace changes. The optical designer should be aware of what departures $n(\lambda)$ has taken from $n_0(\lambda)$ so that a proper choice of variables may be made.

II. Methods

When fabricating diffraction-limited objectives, optical glass is typically purchased to a much more liberal tolerance than what is required for fabrication. For example, when procuring the material it may be required that n_d be within ± 0.001000 of the catalog nominal, yet the actual index must often be known to ± 0.000010 for successful fabrication of the objective. This large disparity between the accuracy needed by the glass vendor, and that of the end user often makes it necessary for the end user to have index of refraction measurement capability. Such was the case for our Company. In sponsoring this research, Melles Griot has refurbished a spectrometer that is capable of measuring refractive index to the fifth decimal place.

• Experimental Equipment

A spectrometer is a precision instrument that is used to measure prism angles and deviation angles of light which passes through a prism. Of prime importance in any spectrometer is the circular reference scale which is divided into degrees, arc minutes, or arc seconds. For this research, an old Gaertner L123 spectrometer was acquired. The steel reference scale is 7 inches in diameter and is engraved every 10 arc minutes. With the aid of its microscopes and filar eyepieces, it is able to measure prism angle to ± 5 arc seconds* [see Appendix 3, page 76], minimum deviation angle to ± 5 arc seconds, and, therefore, refractive index to ± 0.000025 [for n = 1.65; see Appendix 4, page 85].

The spectrometer is shown in Figure 5. The sample is prepared in the shape of a prism and placed on the platform above the rotation axis of the instrument. Spectral lamps are placed at the slit aperture of the collimator, located to the right. The radiation is collimated and passed through the prism sample. After emerging from the sample, it is still collimated, though deviated by refraction. The observation telescope is swung about its axis until the radiation enters its aperture whereupon the

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* The difference of two measurements of rotational position are required. Each is accurate to ± 2.5 arc seconds.

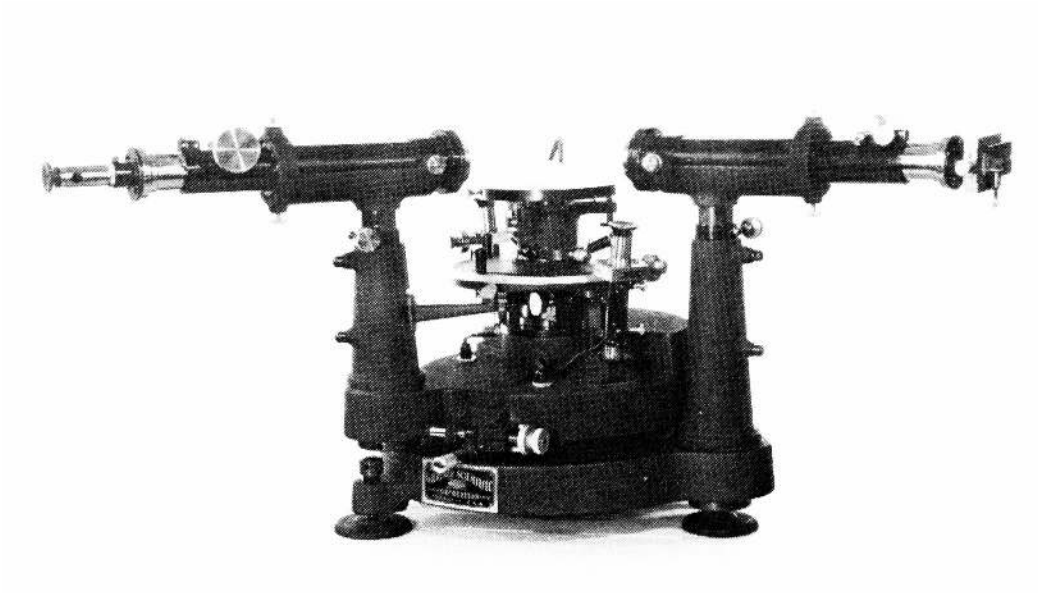

Figure 5 Gaertner L123 Spectrometer

slit is now visible with the aid of the eyepiece. As the observation telescope is pivoted, the two microscopes which permit viewing of the circular scale move with it. By subtracting the scale reading obtained when the sample is in place, from the reading obtained when the sample is withdrawn, the angular deviation of the radiation due to the prism is determined. If the prism angle is measured carefully, and the angle of incidence that the radiation makes with the prism face is known (directly or indirectly), then the refractive index of the sample at the wavelength of the spectral lamp may be determined [see page 33].

Various elemental spectral lamps are used as radiation sources. Each emits characteristic line spectra at wavelengths known to high precision.[53,54] Over the wavelength interval of interest, a set of spectral lines is chosen and the test sequence described above is performed. A table of refractive indices at these test wavelengths results. These data are used as the basis of further analysis, in which experimental errors are smoothed, and interpolation of index at wavelengths other than the test wavelengths is allowed. Special software has been written to perform these analyses.

• Software

Two categories of software were written. The first assists with data acquisition when operating the spectrometer; a Hewlett-Packard 41C programmable, hand-held calculator is used. Actual analysis and curve-fitting is performed by a program written in Fortran for the MS-DOS or VAX/VMS environment.

ATON *Angle to Index*; This HP-41C program is the front-end for the other two programs. It provides the user interface for reducing the data from the spectrometer to prism angles, minimum deviation angles, and refractive index. It also shows the difference between microscope readings of the divided circle so that potential reading errors can be spotted.

SAD *Spectrometer Angle and Difference*; Takes the two microscope readings of the divided circles, in degrees, minutes, and seconds, and determines the average reading and the difference of this average with the last average.

ADN *Prism Angle A, Minimum Deviation Angle D, and Refractive Index N*; Written in the interchangeable solution format where you supply any two of the parameters and the third is computed. ATON sets up A and D as known parameters and N is solved for. As a stand-alone program, ADN is useful for running *what if?* problems where prism angle A is perturbed slightly and the effect on index N is noted.

When using the spectrometer, the data is reduced immediately from microscope readings of the divided circle to prism angle and minimum deviation angles so that ATON's diagnostics can be used to spot any potential misreading of the divided circle or filar eyepieces. The design of the filar eyepieces makes reading errors of 1 arc minute likely. Errors of 10 arc minutes are less likely, though possible. The diagnostics provided by these programs minimize the chance that erroneous data will go undetected at the time of test. The Fortran-based analysis software MELT would detect the erroneous data, but, if postponed until analysis, corrected data may be more difficult to obtain. It is best to do some data checking as the experiment is being performed.

The task of the Fortran program MELT is more complex. Figure 6 shows, in the form of a flow chart, the general procedure.

First, the experimental data are read from files and/or the keyboard. Commands that instruct MELT what to do with the data are input. It then carries them out without further input.

For each data point, the experimental wavelength, observed refractive index, experimental uncertainty that should be assigned to the index, and the nominal (expected) index is specified. Of the four, only the first two are required. Uncertainty, if specified, is used to weight data in proportion to its precision during curve-fitting. Any specified nominal index is used in preference to the calculated value that MELT supplies. See page 106 for the input data syntax.

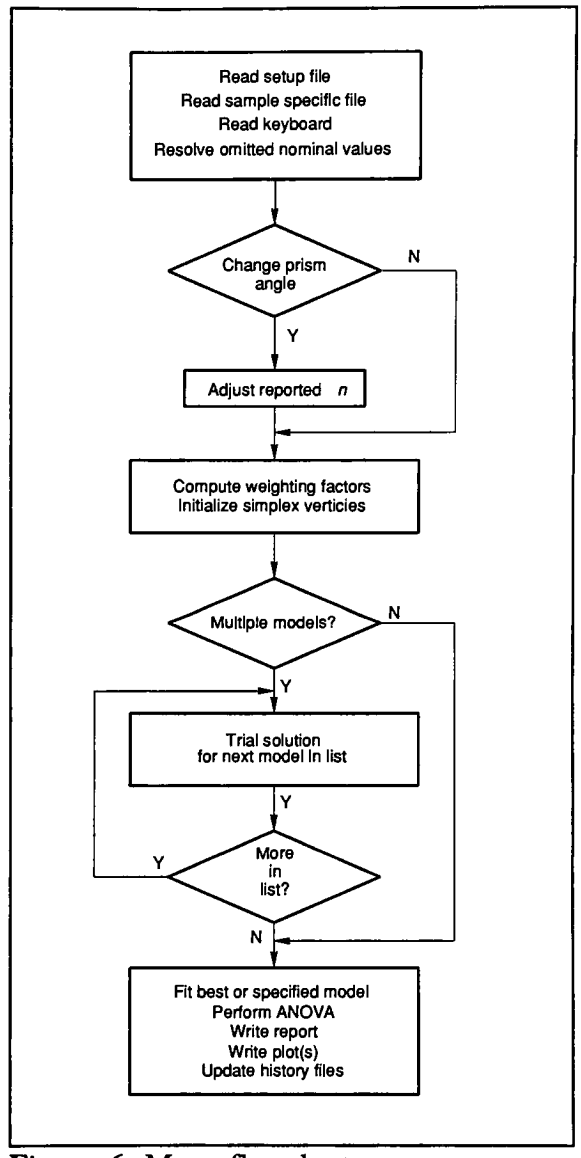

Figure 6 MELT flowchart

After all input of data and commands, MELT fits the specified model to the experimental data and analyzes the results. If the model relies on a nominal dispersion function $n_0(\lambda)$ then the manufacturers' catalogues will be used to resolve any omissions that the user may have made in providing nominal values. This is normally how the nominal indices are provided; only when the experiment is performed at wavelengths where the manufacturers' dispersion formula is invalid, or when the material under test does not have coefficients for $n_0(\lambda)$ on file, are nominal indices explicitly stated.

Over 30 different models and 4 different merit functions are provided. Some models are composite functions of the manufacturers' nominal dispersion formula, Eq. (2), and some do not involve a nominal dispersion model. The latter are provided for completeness and convenience since MELT is also useful for creating a dispersion model when one is not available in the literature. This is not the subject of this thesis, however. This research relies on a known, nominal dispersion model. Over 20 such models are provided.

The "goodness-of-fit" of the model to the experimental data is judged mathematically with a *merit function*. It measures the agreement between the data and the model for a particular choice of parameters. Four different merit functions are provided, each formulated so that small values represent close agreement between the data and the model. Guidelines for using one in preference to another are given on page 46.

Weighted sum of squares

$$f = \sum_{j=1}^{j_{\max}} w_j^2 \left[n_j - n\left(\lambda_j;\ b_1, b_2, \ldots, b_{k_{\max}}\right) \right]^2 \tag{20}$$

Weighted sum of absolute

$$f = \sum_{j=1}^{j_{\max}} w_j \left| n_j - n\left(\lambda_j;\ b_1, b_2, \ldots, b_{k_{\max}}\right) \right| \tag{21}$$

Weighted maximum deviation

$$f = \max \left[w_j \left| n_j - n\left(\lambda_j;\ b_1, b_2, \ldots, b_{k_{\max}}\right) \right| \right] \tag{22}$$

Chi-square

$$f = \sum_{j=1}^{j_{max}} \left[\frac{n_j - n\left(\lambda_j;\ b_1, b_2, ..., b_{k_{max}}\right)}{\Delta n_j} \right]^2 \qquad (23)$$

The term n_j is the observed response, and $n(\lambda_j; b_1, b_2, ..., b_{k_{max}})$ is the model's response. The w_j factor is the weight assigned to the jth data point, and is equal to the reciprocal relative Δn (the point with the smallest Δn in the data set has a weight of unity, and all others have a smaller weight). Data points having the smallest stated uncertainty, Δn,* have the greatest potential for impacting the value of the merit function. The model $n(\lambda_j; b_1, b_2, ..., b_{k_{max}})$ is a function of wavelength λ, and parametric in the coefficients $b_1, b_2, ..., b_{k_{max}}$ which MELT seeks to determine. This model may be linear or highly nonlinear in these coefficients. Minimizing the value of the merit function implies optimizing the model to the data.

The minimization method used by MELT is the *downhill simplex algorithm*** of Nelder & Mead.[55,56] It does not require knowledge of derivatives—only function evaluations are required. It adapts to the function f being minimized by reflection, extension, contraction, or shrinkage of the simplex in response to characteristics of the surface.

A simplex is a geometric figure that has one more vertex than the space in which it is defined has dimensions.[57] On a plane, which is a two-dimensional space, a simplex would be a triangle; in three-dimensional space it would be a tetrahedron. The function f being minimized describes a surface. It is evaluated at the vertices of the simplex. The vertices are ranked from best to worst, and the worst is replaced with a better estimate by moving away from the high function value that it represents. In this way, the simplex moves towards the function's minimum by moving away

---

* Ideally, Δn_j is the standard deviation of the estimate of n_j, σ_j.

** Not to be confused with the *simplex method of linear programming* where both the function being optimized, and the constraints, happen to be linear functions of the independent variables.

from high values. Most other minimization procedures attempt to move in the direction of the minimum by moving in a straight line towards it,[58] with the fastest algorithms of this type utilizing partial derivatives to point the way. But with this speed comes the possibility of divergence. The simplex algorithm cannot diverge. Though not the most efficient, requiring on the order of j_{max}^2 storage and many more function evaluations than most, its advantages* can easily outweigh its speed disadvantage for jobs were the computational burden is small.

After the merit function f is minimized, the difference between the optimized model $n(\lambda_j; b_1, b_2, ..., b_{k_{max}})$ and the experimental values n_j is evaluated and summarized in tabular, graphical, and statistical form. If the fit of the model to the experimental data is judged by MELT and the analyst to be adequate, the indices that MELT computes for the design wavelengths may then be used for the melt recomputation. By considering the model that was required, the optical designer can often make a better choice of variables: if it is known that the partial dispersion of the material has deviated from its expected value, the designer may allow curve changes. Not knowing this about the material, only airspace changes might have been allowed. This knowledge can save time and lead to a superior fabrication solution.

* It cannot diverge. It is insensitive to initial values—the solution does not need to be surrounded or bracketed as with the *golden section search*, or *Brent's method*. Derivatives do not need to be known or computed numerically, as with *Marquardt's*, *Powell's*, or other methods based on the *Newton-Raphson* algorithm. Almost no special assumptions are made about the nonlinear function being minimized. It is not necessary to linearize it by variable transformations, which can lead to undesirable weighting. Though not needed for this application, the function being minimized may be formulated so that the simplex stays out of certain solution areas [Olsson, p. 45 (ref. 58)]. This *constrained optimization* may be accomplished by adding a penalty term to the function, or by transformation of the bounded space into an unbounded one.

III. Results

To examine the behavior of a large number of samples, it was necessary to write flexible software, sophisticated enough so that it is easily used in a production environment. The results of many trials with different interpolation models are summarized in this Section; greater detail is presented in Section IV.

• The Effect of Annealing on Dispersion

No reason has been found to reject the null hypothesis H_0 in favor of the alternate hypothesis H_1 [see page 15]. Multiple annealings of material from the same melt have always been observed to have parallel dispersion functions $n(\lambda)$ that are simply shifted in the direction of the ordinate n from one another.

This does not constitute proof of H_0 but, rather, lack of disproof. As is often the case, H_0 is difficult to prove but easy to disprove with only a single counter-example. Such an example has not been encountered. Rejection of H_0 is not required on the basis of the data collected and reviewed.

• MELT Makes Subtle Differentiations

Although H_0 has not been disproven, this is not to say that all samples have been observed to have their $n(\lambda)$ curve parallel to the nominal $n_0(\lambda)$ curve. Indeed, some have been different enough from their expected curve shape that they should be classified as separate and distinct glass types! Spotting curve shape changes is difficult without MELT. If the designer fails to realize that such a material is planned for use in fabrication, an inappropriate choice of variables may be made during the melt recomputation.

MELT has been instrumental in spotting substitutions of "equivalent" glass types by well-meaning vendors. For example, Schott LaFN-2 and LaF-2 are considered equivalent since their n_d and V_d values are the same; the rate of change of index

with wavelength, $dn/d\lambda$, is not.* LaFN-2 is called for in a fast, complicated, diffraction-limited objective that is intended for usage at a laser wavelength and a nearby, broad wavelength interval. The objective is particularly intolerant of changes in the derivative of index with respect to wavelength, yet very tolerant of shifts of the dispersion function $n(\lambda)$ in the direction of the ordinate n. The vendor's data sheet indicated that the material was LaFN-2, though analysis performed by MELT clearly indicates that it is LaF-2. If this had not been recognized, many hours may have been wasted trying to perform the melt recomputation using ineffective variables.

• Recommended Interpolation Model

The refractive index of optical glass is a very nonlinear function of wavelength. Expressed as a function of frequency, υ, it is more linear. It should not be surprising, then, that the simplest interpolation models are those which involve reciprocal wavelength terms since frequency and wavelength have the reciprocal relationship

$$\lambda = \frac{c}{\upsilon} \quad , \qquad \text{where} \quad c = 3.0 \text{x} 10^8 \text{m/s} \quad . \tag{24}$$

Best results are obtained when a composite function is formed of the nominal dispersion model for the material under test, $n_0(\lambda)$, and one or more perturbation terms. As recommended on page 13 of the Introduction section, the manufacturers' dispersion model, Eq. (2), is used as this nominal model. The perturbation terms represent the departure of the actual material from the nominal material.

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* Comparing the relative partial dispersions of LaFN-2 and LaF-2 is also a useful method of telling the two apart. It is not necessary to examine the derivative, $dn/d\lambda$. The relative partial dispersion $P_{x,y}$ may be defined as

$$P_{x,y} = \frac{n_x - n_y}{n_F - n_C} \quad .$$

Both LaFN-2 and LaF-2 have the same principal dispersion n_F-n_C, and the same n_d value, but the dispersion between arbitrary wavelengths x and y is not the same.

The least complex perturbation would be

$$n(\lambda) = n_0(\lambda) + B_1 \tag{25}$$

which would simply translate the nominal model n_0 in the direction of the ordinate n. More complicated departures from nominal are possible; the following models are recommended and should be applied in order of increasing complexity:

$$n(\lambda) = n_0(\lambda) + B_1 + \frac{B_2}{\lambda} \tag{26}$$

$$n(\lambda) = n_0(\lambda) + B_1 + \frac{B_2}{\lambda^2} \tag{27}$$

$$n(\lambda) = n_0(\lambda) + B_1 + \frac{B_2}{\lambda^{B_3}} \tag{28}$$

$$n(\lambda) = n_0(\lambda) + B_1 + B_2\lambda^2 + \frac{B_3}{\lambda^2} \tag{29}$$

The output from MELT can be used to decide when the model complexity should be changed. Generally, the simpler the model the better. Allowing too many degrees of freedom may lead to unwarranted changes in curve shape and should be avoided, as discussed on page 14.

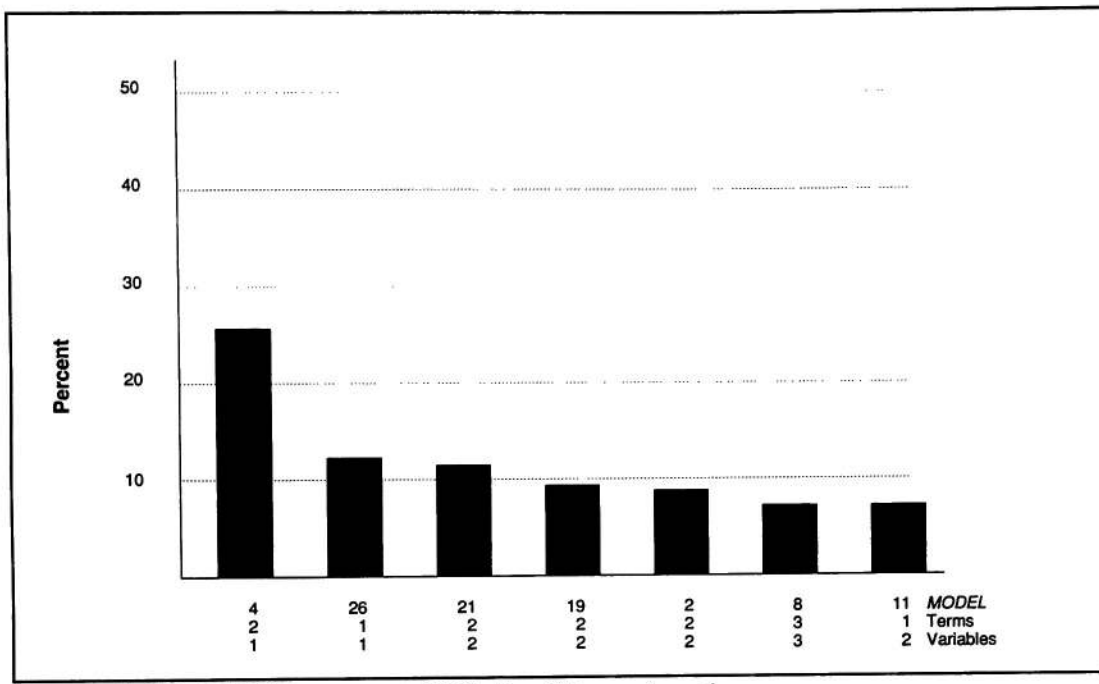

Figure 7 Model Histogram at 95% Confidence Level

MELT should first be run using Eq. (26)* as the interpolation model. The problem is then rerun using Eq. (27)** as the model; then Eq. (28)*** is used (and so on). To decide which is best, the value of the "*F* TEST FOR SIGNIFICANCE OF THE REGRESSION TERMS EXCLUDING THE MEAN" is examined. Beginning with the least complex model, this *F* test will increase to a peak value as the optimum interpolation model is reached, and then decline as the model becomes too complex. If the *F* test is always increasing (never peaks), then more complexity may be

* The MELT command is *MODEL 2.*

** The MELT command is *MODEL 4.*

*** The MELT command is *MODEL 24.*

necessary. If it is always decreasing, then the least complex model may be too complex.

The computed value of the F test must always be greater than or equal to the *critical value* of the F distribution. If it is not, then the term(s) are insignificant and Eq. (25)* is indicated—a single term representing the mean.

MELT may be run so that it examines a list of models and selects the best one based on this criterion.** It will display the merit function and F test values for each one, and then perform the full analysis using the one chosen. This eliminates the need for multiple runs and is the recommended mode of operation.

The histogram presented in Figure 7 summarizes how often a model has been found to be optimum in a production situation. Models 4, 21, 19, and 2 all have two degrees of freedom; model 26 has only one. Clearly, models of minimal complexity are favored.

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* The MELT command is *MODEL 26*.

** The MELT command to examine these models automatically is *MODEL 2 4 24*; an arbitrary number of models may be listed in this fashion. If the F test is always less than the critical value, then the analysis will be performed as if *MODEL 26* had been specified.

IV. Discussion

In the preceding two sections, an overview of the methods by which optical materials are characterized has been offered, and the results of experiments using these methods have been summarized. This section expands on these summaries.

• Experimental Equipment

Refractometers may be broadly grouped into two categories: those which measure by *critical angle* methods, and spectrometer methods which do not. Of these two, the spectrometer is capable of the highest accuracy and precision.* Critical angle methods generally involve less sample preparation and may be accomplished with samples of minimal dimensions. Instruments whose design allows such methods are indispensable tools for the nondestructive testing of work in progress, for the need to quickly determine the index of refraction of small samples frequently arises.

The Pulfrich refractometer operates by critical angle measurement. It only requires that a single surface of a small sample be polished flat. The specimen having unknown index function n is placed in contact with a reference block having known index function N such that $n < N$. Imperfect specimen polish can be accommodated by introducing a liquid of slightly higher index than N between the two. The arrangement is shown in Figure 8.

A diffuse source illuminates the specimen such that some rays strike the boundary of the specimen and the block at grazing incidence. Such rays are refracted at the critical angle into the block; their angle of refraction into the medium of index N may be no larger. The telescope is used

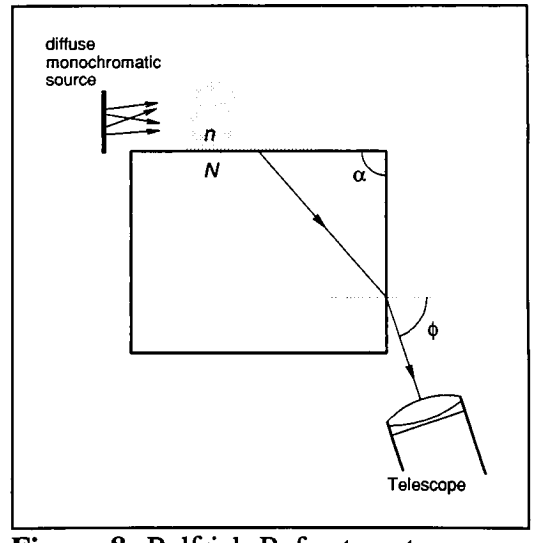

Figure 8 Pulfrich Refractometer

* *Accuracy* has to do with the closeness to the "true" value of the quantity measured; *precision* refers to the closeness together of repeated measurements of the same quantity.

to observe the source by looking through both media. A demarcation line is visible, marking the critical angle boundary. On one side of this line, the field is bright; on the other side, it is dark.

No rays may have angles of emergence greater than ϕ. The telescope is rotated to determine the angle at which the demarcation line occurs. This angle ϕ is a function of λ, and, when several wavelengths are used,[59]

$$n = \sqrt{N^2 - \sin^2\phi} \tag{30}$$

gives the dispersion of the unknown material.

Use of Equation (30) requires that the angle, α, between the two faces of the reference block be precisely 90°. The error introduced if it is not varies with n and N, and can be significant.* The general equation for n, of which Eq. (30) is a special case, allows for circumstances where 90° is not an accurate value for α,[60]

$$n = \sin\alpha\sqrt{N^2 - \sin^2\phi} \; - \cos\alpha \; \sin\phi \quad . \tag{31}$$

A spectrometer may be operated in a manner which duplicates the function of a Pulfrich refractometer. A previously measured prism having known dispersion function N is used as the reference block, chosen such that $n < N$ as before. The spectrometer is used to measure α and ϕ very accurately. Equation (31) yields the index of the specimen, n. This may seem to be a poor utilization of the spectrometer's potential, but production situations occur for which it is impossible to fabricate a sample prism for normal analysis by spectroscopic means.

* As an example: If N is 1.74 and n is 1.58, a five arc second error in the angle α will cause a $\pm$ 0.000020 error in n; if n is 1.70, a five arc second error causes a $\pm$ 0.000090 error in n.

The principle of operation of an Abbe refractometer is the same as that of a Pulfrich. The demarcation line locates the rays entering the reference block at grazing incidence and define an angle of emergence, ϕ. As before, dispersion N and angle α of the reference block must be known. The design of the instrument makes it well suited for the measurement of liquids. It is rarely used for high accuracy measurement of solids.

Critical angle refractometers depend on correct positioning of the eyepiece reticle on the demarcation line separating light and dark areas in the field of view. This lack of symmetry contributes to a reduction in the accuracy that an observer can attain. With a spectrometer, the eyepiece reticle is superimposed on an image of the slit; the viewing symmetry allows for more accurate positioning.

Sample preparation difficulty is a serious drawback of the spectrometer. On a relatively large specimen, two faces must be polished flat to high accuracy. Critical angle measuring refractometers relax the sample preparation burden, but they rely upon the knowledge of the dispersion function N to an accuracy at least five times greater than that desired of n. For measurements into the *6th* decimal place, the reference block must have known dispersion characteristics to an accuracy measured in the *7th* decimal place. This is a tall order indeed!

The Hilger-Chance refractometer (sometimes called a "V-block" refractometer) was developed to avoid some of the drawbacks of both the spectrometer and critical angle measuring devices. This refractometer still relies on the knowledge of the dispersion function N of a reference block, but a slit is observed by the telescope rather than a demarcation line between light and dark. The reference block is made from

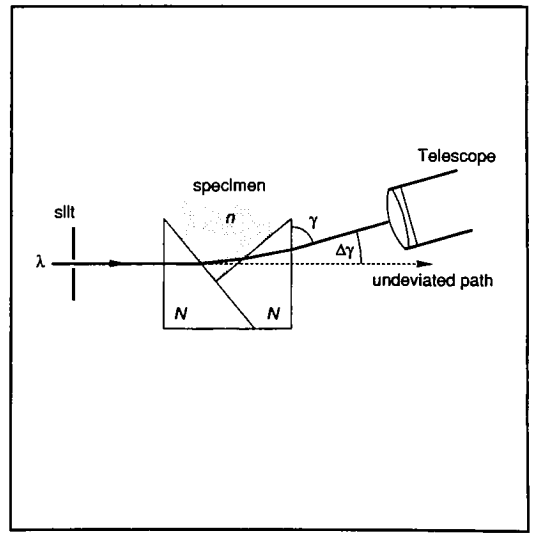

Figure 9 V-block Refractometer

two prisms that were cut from the same material. Figure 9 indicates how they are united to form a V-shaped chamber.

If a specimen having the same refractive index as the block were introduced into the chamber, the ray path would be undeviated. Introducing a sample having a different index deviates the path of the rays. The amount of this angular deviation is used to compute the unknown index n,[61]

$$n = \sqrt{N^2 + \cos\gamma \sqrt{N^2 - \cos^2\gamma}} \quad , \text{ or} \tag{32}$$

$$n = N + \frac{\Delta\gamma}{2} - \frac{\Delta\gamma^2}{8N} - \left(\frac{1}{4N^2} + \frac{1}{12}\right)\Delta\gamma^3 - \cdots \quad . \tag{33}$$

Though it is possible, in principle, to use a single reference block, this is a poor practice. It is best to have many V-block chambers available and, for testing a sample having refractive index n, to choose the reference such that $N \approx n$.* This reduces the method's sensitivity to fabrication errors of the sample, particularly in achieving a 90° angle between the two faces. Index matching fluid may be used to accomodate an imperfect right angle or unpolished surfaces.

As $n \rightarrow N$, $\gamma \rightarrow 90°$ and $\Delta\gamma \rightarrow 0$. The series expansion for Eq. (32), shown as Eq. (33), may be truncated after the third term if the reference is chosen so that $| n\text{-}N | \leq 0.000500$ since $\Delta\gamma \approx 0.001$ radian (further terms are $<< 1 \times 10^{-6}$).[62]

A spectrometer does not require a reference block that has known dispersion properties; its measurements are absolute, rather than relative. Though the test is the most intuitive of all the refractometry methods, it is also the most laborious to perform. Figure 10 and Figure 11 show the test geometry.**

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* Since the device is not measuring critical angle, it is not necessary that the sample index n be less than the reference block index N.

** A photograph of the spectrometer used for this research is shown in Figure 5 on page 16. The unit is more fully described in Appendix 3.

The prism sample is fabricated from the material having unknown refractive index n. Faces AB and AC are ground and polished flat; face BC is not used and may be of arbitrary surface quality. The two polished faces are separated by the *prism angle*, α. A ray incident at face AB at angle I_1 traverses the prism and emerges from face AC at an angle I_2'. The angle D between the initial and final directions of the ray is the *angle of deviation*. It may be shown[63,64] that D is minimized when $I_1 = I_2'$. This is the so called *minimum deviation* condition where rays pass through the prism symmetrically. Minimum deviation may be set to high precision with a spectrometer, which is one of the principal reasons why it allows n to be determined to such high precision.

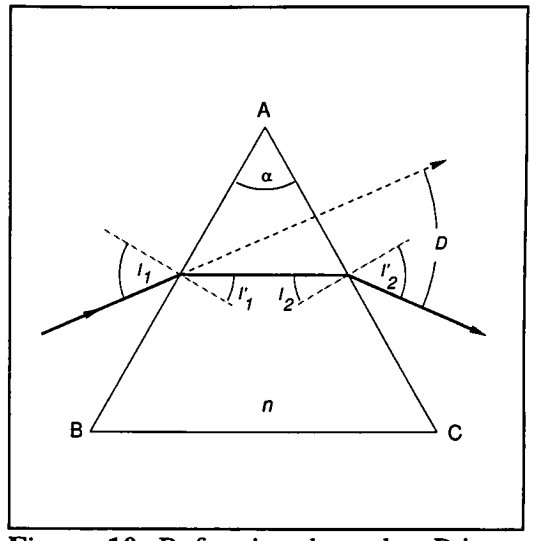

Figure 10 Refraction through a Prism

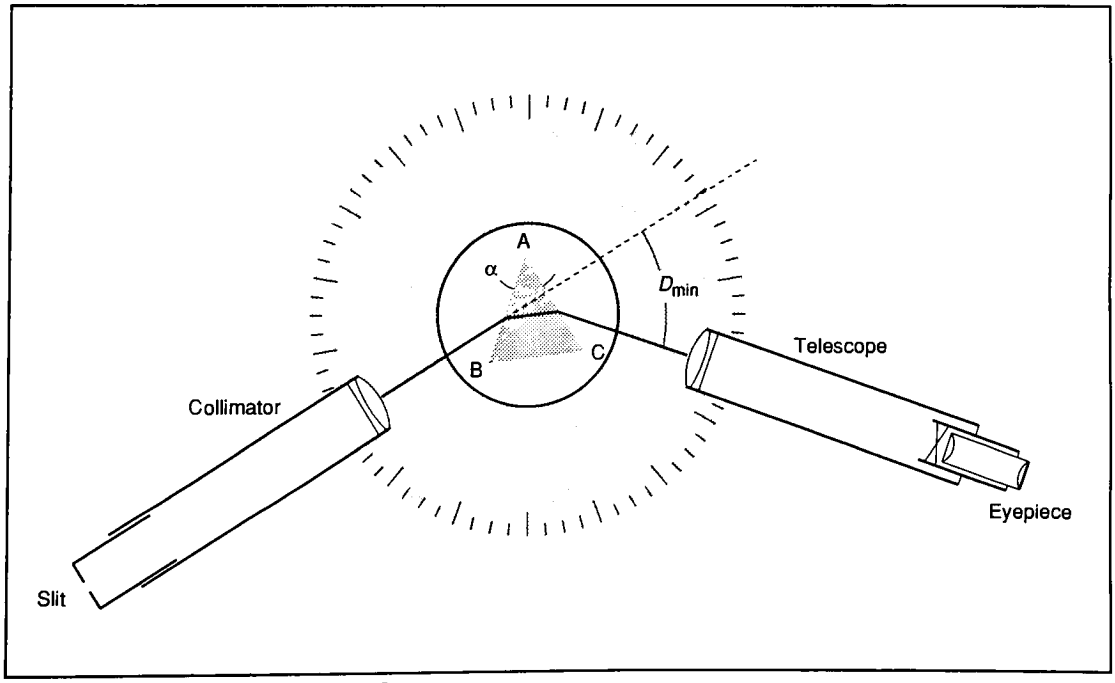

Figure 11 Spectrometer Refractometer

At minimum deviation, $I_1' = I_2 = \alpha/2$, which immediately suggests that a sample of half the size could be used by bisecting the full prism angle α, and by autocollimating off the new face so that the rays retrace their path.[65] With such an autocollimating spectrometer, the angle of incidence I_1 is measured for each λ. The dispersion function n would then be described, using[66]

$$n = \frac{\sin I_1}{\sin \frac{\alpha}{2}} \quad , \tag{34}$$

where $\alpha/2$ is the measured prism angle. But Tilton[67] builds a concrete case for preferring minimum deviation spectrometry over the autocollimation approach based on maximizing the tolerance of angular measurements. Minimum deviation spectrometry does not require the measurement of I_1; the geometry of the condition allows D_{min} to be measured instead, indirectly providing the angle of incidence. When at minimum deviation, the general analytical formula describing the passage of a ray through a prism reduces to the *spectrometer formula*,[68]

$$n = \frac{\sin \frac{\alpha + D_{min}}{2}}{\sin \frac{\alpha}{2}} \quad , \tag{35}$$

which is identical to Eq. (34) when it is recognized that

$$I_1 = I_2' - \frac{D_{min} + \alpha}{2} \quad . \tag{36}$$

The errors which occur in the practice of precise prism refractometry may be classified into two categories: First, having to do with the prism sample and its

relationship to the spectrometer; second, having to do with the spectrometer only, and its use as a goniometer. These two sources will be considered in turn.

Total internal reflection will occur if the prism angle is made too large. This constraint may be expressed as

$$\alpha < 2\arcsin\frac{1}{n} \quad . \qquad (37)$$

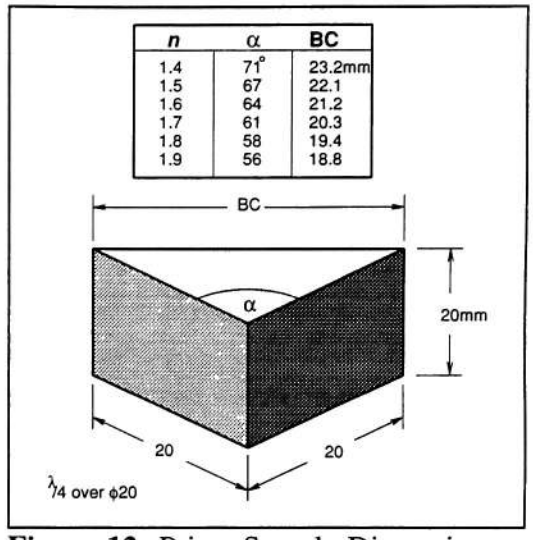

Figure 12 Prism Sample Dimensions

As this limit is approached, the intensity of the slit image will be greatly reduced, and a serious increase in aberration will occur.

Less obvious are the constraints on angle measurement tolerance. The value chosen for α has a strong influence on whether the full precision and accuracy of the spectrometer are attained. By adhering to the careful sample design described below, the full potential of the device may be realized.

Determination of index to $\pm$ 0.000010 accuracy requires that α and D_{min} be measured on the order of arc seconds. The tolerance can be relaxed on these angular measurements, while minimizing the uncertainty in computed index, by optimum sample design. Tilton[69] has performed the definitive error analysis of minimum deviation refractometry. Examination of the partial derivative of the spectrometer formula, Eq. (35), with respect to prism angle α, and then with respect to deviation angle D (in the neighborhood of D_{min}),

$$\frac{\partial n}{\partial \alpha} = -\frac{\sin\frac{D}{2}}{2\sin^2\frac{\alpha}{2}} \quad , \text{ and} \tag{38}$$

$$\frac{\partial n}{\partial D} = \frac{n}{2\tan\frac{\alpha+D}{2}} = \frac{\cos\frac{\alpha+D}{2}}{2\sin\frac{\alpha}{2}} \quad , \tag{39}$$

leads to the conclusion that the optimum prism angle, α_0, is a function of the sample's index n. It may be expressed as

$$\alpha_0 = 2\arctan\frac{1}{n} \quad . \tag{40}$$

The tolerance on the measurement of D_{min} is relaxed slightly by fabricating α slightly larger than α_0, but this will make the measurement of α more difficult.* Fabricating the prism angle less than α_0 also increases the difficulty in measuring α, and it makes the measurement of D_{min} more difficult too. As n increases, not only is it more important to adhere to Eq. (40), but the precise measurement of α is much more important also.**

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* Such a strategy might be appropriate if precise determination of partial dispersions is desired, even at the sacrifice of accuracy in the magnitude of n.

** The data reported by Tilton (p. 921, reference 67) indicates, for example, that it is necessary to measure α to ± 2.7 arc seconds if the impact on the computed index is to be less than ± 0.000010 for a prism having n of 1.5, fabricated with α of 45°. If fabricated with α of 67.4° ($=\alpha_0$), the measurement tolerance for α is increased to ± 3.3 arc seconds—an increase of almost 25%. For n of 1.75, a 45° value for α requires that α be measured to ± 1.7 arc seconds; using α_0 of 60°, the tolerance is ± 2.0 arc sec—only an 18% improvement.

The last considerations for optimum sample design have to do with the size and polish of the two faces. Figure 12 summarizes the optimum sample size requirements. Tilton[70] has tested the presumption that larger prisms allow greater accuracy and reports that no significant improvement in the pointing accuracy of the spectrometer was obtained by using prism face dimensions larger than those shown. Square faces are strongly preferred to rectangular ones of the same area, however. The magnitude of n is inconsequential.

The polish of the two faces is also generally recognized as "important". Again, Tilton[71] has quantified the requirements,* finding them to be not as stringent as widely held. If it is desired that the curvature contribute less than ± 0.000001 uncertainty in the computed index, and samples are of the dimensions shown in Figure 12, $\lambda/4$ surfaces are perfectly acceptable. Face curvature makes it necessary to decollimate the spectrometer's observation telescope during the measurement of the prism angle, α. A compromise focus setting must be made—it is not possible to optimize the focus setting for each face. Polish is more important if the prism is not "well-tabled," in Tilton's words. By this he means that the prism's two faces must be well centered (± 0.1 mm) in the telescope's field. It is important to use the same region of the faces for the autocollimation measurement of the prism angle α, and refraction angle D_{min}. Any residual curvature of the prism faces will locally perturb the value of α and influence the computed value of n. Appendix 5 [page 87] discusses the impact of face curvature on the measured prism angle α in detail.

The direct contributions of the spectrometer to the uncertainty in the computed index will now be considered. Closely related to the sample's face curvature is the collimator's focus setting. If the collimator is set incorrectly, then the telescope must be decollimated to compensate. This will reduce the accuracy to which α may be

* The curvature which will cause a ± 0.000001 error in the computed index n is a function of the magnitude of n. For a sample having an index of 1.5, and α of 67°, the curvature must be $\leq \lambda/8$ over a 10 mm diameter (λ = 0.5461 μm; over 20 mm this would be $\lambda/2$). For n of 1.75 and α of 60°, the curvature must be $\leq \lambda/15$ over 10 mm ($\lambda/4$ over 20 mm).

determined by autocollimation off faces *AB* and *AC*. Further, collimation should be set in the middle of the wavelength range that is expected so that the impact of residual longitudinal chromatic aberration of the collimator is minimized (collimation will vary with wavelength). The tolerances given by Tilton[72] are within the capabilities of devices constructed with an *f*/10 achromatic doublet, which would require a reasonable 15 inch tube length to produce a 1.5 inch diameter beam.*

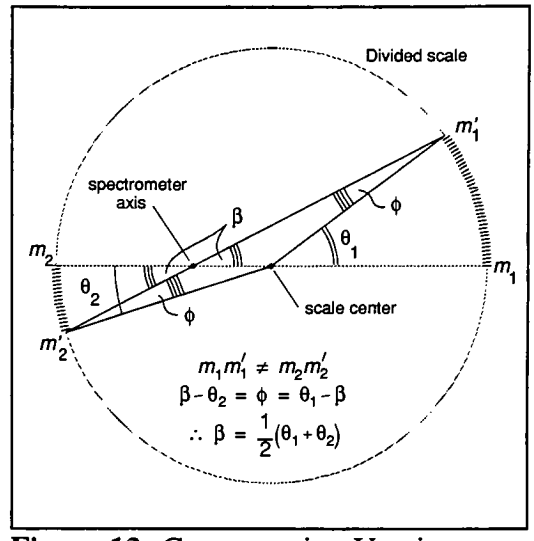

Figure 13 Compensating Verniers

The design of the spectrometer makes it possible to eliminate a further source of error that afflicts all goniometric devices. If the center of the divided circle is not intersected by the rotational axis of the instrument, the angles read from the divided circle will be erroneous. It is impossible, from a practical standpoint, to center the scale with the bearing (at the time of manufacture) to the accuracy necessary for the impact on the angular readings to be negligible. It is simple, however, to compensate for the small, but inevitable decentration that is intrinsic with the device, or which develops over time. Multiple microscopes are used to examine the divided scale in diametrically opposite locations.** Figure 13 shows the case where two are used, 180°

* To impact the computed index by ± 0.000001 or less, Tilton recommends that the longitudinal chromatic aberration of the collimator, Δf_c, be less than K times the square of the collimator's focal length, f_c. When expressed in units of millimeters, K ranges from ± 14 x 10^{-6} for n of 1.5 and α of 67°, to ± 12 x 10^{-6} for n of 1.75 and α of 60°.

** Some spectrometers only have one measurement microscope, yet they are utilized for *precision* experimentation. This practice seems contrary to well-established knowledge regarding such instruments. The finest spectrometers for precision minimum-deviation refractometry possess four measurement microscopes rather than two.

apart. It can be shown[73,74] that the simple average of the two readings is free of error that would otherwise occur.

When readings to one arc second are required, consideration must be given to the divided scale markings themselves. Engraving errors may be classified as periodic (systematic) and accidental (irregular). For one arc second precision, these errors are not negligible.

The periodic errors are usually low frequency and can be corrected by developing a Fourier series that is based on the examination of a limited number of divisions. Tilton[75] should be consulted for additional information. High frequency, accidental errors cannot be compensated for by applying a simple correction formula. It is necessary to replicate the readings on various parts of the divided circle and include all of the redundant readings in the data reduction. It will be shown [page 62] that replicated data also serves as the basis for determining whether or not the interpolation model is inadequate.

At least 20 sources of potential error exist when performing minimum-deviation refractometry. Many have limited impact on *6th* place refractometry, leaving five or fewer that restrict the precision and accuracy of the computed index. There are fewer still that impede *5th* place refractometry. All sources, except the prism orientation at D_{min}, are equally likely to cause positive or negative error contributions to the final index.

The error in the angle D_{min} will tend to be on the positive side rather than the negative. This will cause positive error in the computed index. Specific types of eyepieces and operating procedures may be employed to minimize this occurrence; Appendix 3 [page 76] fully describes the particular spectrometer that was utilized and its devices (both hardware and procedural) for minimizing error contributions to the computed index.

• Software

Two categories of software were described on page 18 of the Methods Section. Discussion of the supporting data acquisition software may be found in Appendix 6 [page 92]. The present section will discuss the analysis software named MELT.

An overview of MELT may be found in the Methods Section [page 19]. The goal of the software is to provide highly accurate estimates of the refractive index n at any arbitrary wavelength λ. To this end, special attention is given to model selection and curve fitting procedures.

The current state-of-the-art fits one of the general dispersion formulas reviewed in the Introduction Section [pages 6, 8] to the experimental data. MELT avoids this practice; it fits the nominal curve of the glass type under test to the experimental data instead. This is desirable since it maintains the shape of the dispersion curve that is characteristic of the material, $n_0(\lambda)$, rather than allowing $n(\lambda)$ to freely take on any curve shape that seemed to suit the data. In this way, the enormous amount of data provided by the glass manufacturers is utilized instead of ignored.

Interpolation is preferred, but because of the low-order terms and few variables, extrapolation may be performed with greater reliability than with other methods. A small data set may be used to define a dispersion curve for the sample under test, $n(\lambda)$, and still provide the complicated, nonlinear curve shape that is characteristic of the material. Whether interpolating or extrapolating, it is important to have a measure of the uncertainty in the estimate of n. MELT provides interval estimates as well as point estimates so that the impact of the uncertainty in the data set on the computed values of n may be seen at arbitrary λ values of interest.

• Output

Figure 14 shows an example of plotted output generated by MELT. Information is displayed in several ways. The plot at the bottom of the page shows the nominal dispersion function, $n_0(\lambda)$, and the sample's dispersion function, $n(\lambda)$, as a solid line

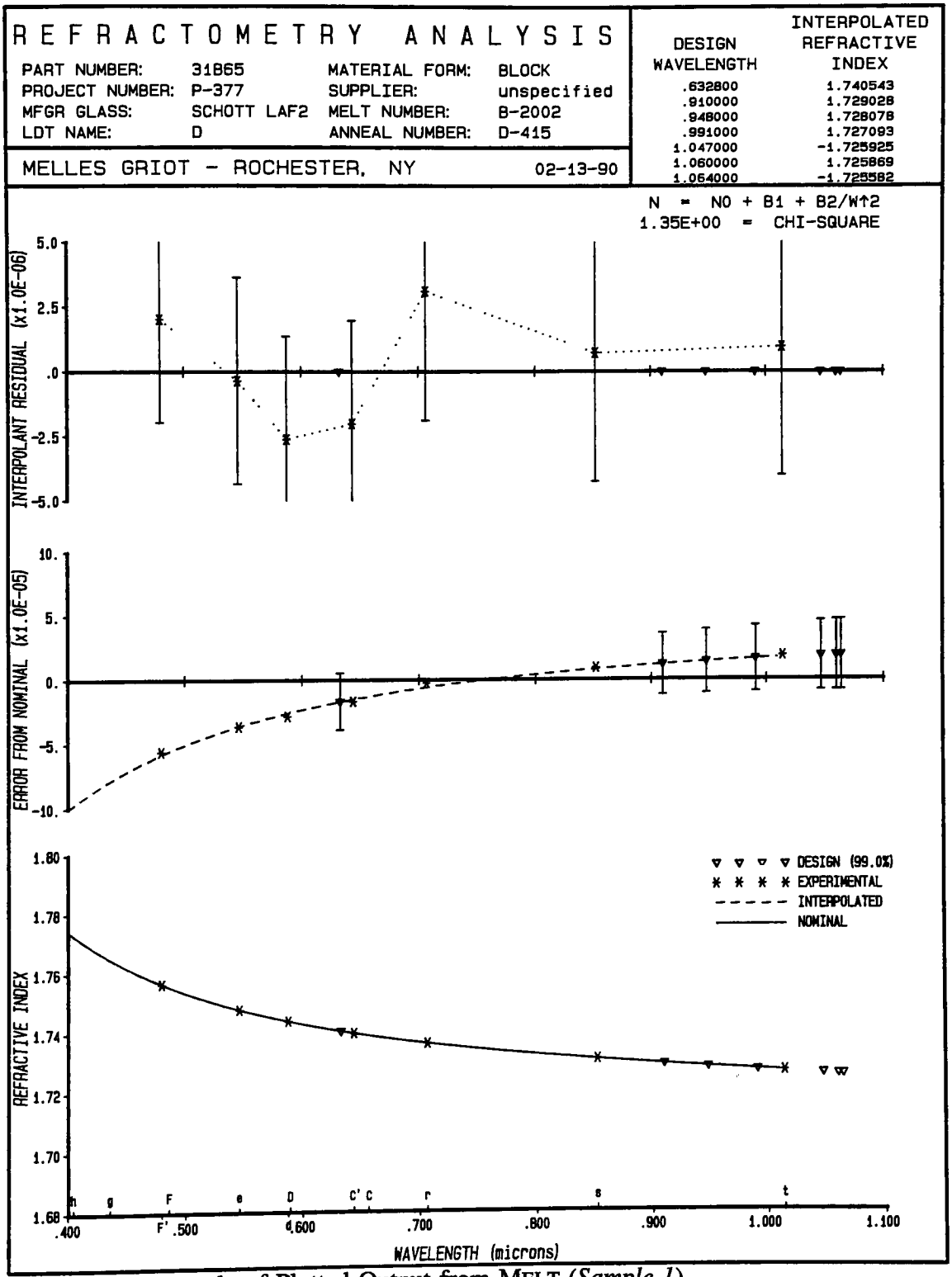

Figure 14 Example of Plotted Output from MELT (*Sample 1*)

and dashed line, respectively.* The locations of the experimental data points are indicated with an "*" character. The "∇" symbol indicates the location of the points that are computed (interpolated or extrapolated) at the design wavelengths. The solid and dashed lines are only drawn for the domain over which $n_0(\lambda)$ is defined as a reminder that estimates of n, at locations indicated by ∇, should be reviewed carefully when made in regions where n_0 is not defined.**

In the upper right-hand corner, the numeric values are given for the points labeled with ∇. Negative values for n indicate that the domain of n_0 has been violated. Values for n_0 may be given at discrete locations in the input file, when such information is available, for the nominal behavior of the glass type (this accounts for the fact that the solid and dashed lines vanish for $\lambda > \lambda_t$, yet the tabulated value for $n_{1.06\ \mu m}$ is positive rather than negative).

The plot in the middle of the page shows the difference between the sample's dispersion and the nominal dispersion, n-n_0. If the sample were identical to the nominal, it would plot directly on the abscissa. If both had identical partial dispersions, the dashed line representing the sample would be parallel to the abscissa though, perhaps, displaced vertically in the direction of the ordinate.

The plot at the top of Figure 14 shows the difference between the experimental points (*) and the model representing the sample's dispersion, $n(\lambda)$.*** It is desired that these *residuals* appear random, and be of a magnitude that is the same as the experimental uncertainties. If a trend (constant upward or downward slope), or some

---

* This particular plot, and the printed output that is associated with it [Figure 15], is for a sample of Schott LaF-2 glass. As mentioned on page 23, the supplier had reported that the material was LaFN-2.

** This kind of extrapolation is unreliable and should be avoided since the error in n_0 may exceed ± 0.000005, and will directly impact the estimate of n.

*** Just as the middle plot may be thought of as the difference between the two lines in the plot just below it, so too may the top plot be thought of as the difference between the "*" and the dashed line in the plot just below it.

R E F R A C T O M E T R Y A N A L Y S I S

PART NUMBER:	31865	MATERIAL FORM:	BLOCK	MODEL NUM:	4
PROJECT NUMBER:	P-377	SUPPLIER:	unspecified	MFTYPE NUM:	4
MANUFACTURER:	SCHOTT	MELT NUMBER:	B-2002	ITERATIONS:	38
GLASS TYPE:	LAF2	ANNEAL NUMBER:	D-415	MERIT:	1.4E+00
LOT NAME:	D	ANALYSIS DATE:	02-13-90	CONVERGENCE:	1.0E-04

DESIGN WAVELENGTH	INTERPOLATED INDEX	NOMINAL INDEX	ERROR FROM NOMINAL	+/- 99.0% CONFIDENCE INTERVALS
.632800	1.740543	1.740560	-.000017	.000022
.910000	1.729028	1.729016	.000012	.000024
.948000	1.728078	1.728064	.000014	.000025
.991000	1.727093	1.727076	.000016	.000026
1.047000	-1.725925	-1.725906	.000019	.000027
1.060000	1.725669	1.725650	.000019	.000028
1.064000	-1.725592	-1.725572	.000019	.000028

WARNING A negative value indicates that a domain violation has occurred for the NOMINAL function. The error may exceed +/- .000005.

EXPERIMENTAL WAVELENGTH	OBSERVED INDEX	INTERPOLATED INDEX	RESIDUAL	+/- 99.0% CONFIDENCE INTERVALS
.479991(F')	1.756603	1.756601	.000002	.000024
.546074(e)	1.747920	1.747920	.000000	.000023
.587562(d)	1.743973	1.743976	-.000003	.000023
.643847(C')	1.739810	1.739812	-.000002	.000022
.706519(r)	1.736278	1.736275	.000003	.000022
.852110(s)	1.730658	1.730657	.000001	.000023
1.013980(t)	1.726600	1.726599	.000001	.000026

EXPERIMENTAL WAVELENGTH	OBSERVED INDEX	NOMINAL INDEX	ERROR FROM NOMINAL	STATED EXPERIMENTAL UNCERTAINTY	MERIT FUNCTION WEIGHT
.479991(F')	1.756603	1.756659	-.000056	.000004	1.000000
.546074(e)	1.747920	1.747956	-.000036	.000004	1.000000
.587562(d)	1.743973	1.744001	-.000028	.000004	1.000000
.643847(C')	1.739810	1.739827	-.000017	.000004	1.000000
.706519(r)	1.736278	1.736281	-.000003	.000005	.800000
.852110(s)	1.730658	1.730649	.000009	.000005	.800000
1.013980(t)	1.726600	1.726582	.000018	.000005	.800000

A N A L Y S I S O F V A R I A N C E

SOURCES	RELATIVE SS	DF	MS=SS/DF
TOTAL (UNCORRECTED)	1.000000	7	
REGRESSION (DUE TO THE MEAN)	.364335	1	2.11948E-09
TOTAL (CORRECTED FOR THE MEAN)	.635665	6	6.16319E-10
REGRESSION (EXCLUDING THE MEAN)	.631945	1	3.67627E-09
RESIDUAL	.003720	5	4.32842E-12

Figure 15 Example of Printed Output from MELT (*Sample 1*)

other functional relationship (parabolic ones are common) appears to be present, then the model used for $n(\lambda)$ is not valid. Randomness is tested by an *analysis of variance*, described on page 50.

Ordinate scales on the top and middle plots are adjusted in magnitude to show detail in the data, so attention should be paid to the labeling. In this example, although the partial dispersion is not the same as that of the nominal glass, note that the range covered by the middle plot is ± 0.000100; the departure was important for the intended usage of this material, but this is not to say that this lack of parallelism is an indication of significant anomalous behavior for every application.

The vertical scale is not expanded or contracted on the bottom plot from one sample to the next. A 0.14 range in n is always shown; the window is simply slid up and down in magnitude. The abscissa may be either wavelength or frequency. Scaling is controlled through commands in the input file, or command entry from the keyboard.

Error bars are shown when the ordinate scale is appropriate. For experimental points (*), these bars represent the stated uncertainty in the reported index. For design points (∇), they are the interval estimates surrounding the point estimates. The printed output may be consulted to determine the exact magnitude of these intervals.

Figure 15 shows the numeric data that is the basis of the plotted output of Figure 14. The layout is similar in both. In the first table is the data for the upper right-hand corner of the plot; in the next table is for the top plot; the third table of Figure 15 contains the data for the middle and bottom plot of Figure 14. The analysis of variance section of the output which follows is described on page 50.

• Input

The input file that MELT reads to produce Figure 14 and Figure 15 is shown in Figure 16. MELT's command interpreter recognizes the keywords and syntax given in Appendix 7 [page 100]. Comments are preceded by a "!" character. The sample is identified, the design λ values are specified, the abscissa scaling is defined, and any

default experimental uncertainty for n is given. Then the experimental data are specified: Between the *BEGIN DATA* and *END* are records with the experimental λ, n, Δn, and n_0 specified. If Δn is omitted for any λ, the default value previously defined is used. If n_0 is omitted, the table between the *BEGIN NOMINAL* and *END* is searched; the manufacturers' dispersion formula is used if any n_0 values remain unresolved. Files of this type are created on a sample-by-sample basis.

Before reading this sample-specific file, a setup file is read. This file, MELT.MEL, is shown in Figure 17 and Figure 18. It is from this file that any installation-specific instructions are read, and the default operating characteristics are set. Text describing each of the models is given between *BEGIN FORMULAS* and *END*. The locations of supporting files are specified, defaults are established for printing and plotting, and then optimization controls are set. MELT will evaluate a list of models, or use a specific model, depending on whether a list of model numbers is

```
! PN31865D.MEL   -   P/N 31860, Summer 1988 build.

PART_NUMBER     31865
PROJECT_NUMBER P-377
GLASS_TYPE      LAF2  ! (supplier's sheet said this was LAFN2)
LOT             D
MELT            B-2002
ANNEAL          D-415
FORM            BLOCK
MANUFACTURER    SCHOTT
WAVELENGTHS     1.064  .948 .910 .991 1.060 1.047  ! ...the "design" wavelengths.
MAX             1.1
MIN             .4

! Schott "High-Precision Readings".
uncertainty     .000005  ! Default experimental uncertainty if not explicitly stated.

BEGIN DATA   ! wavelength, observed_index [, index_uncertainty [, nominal_index ] ]
d       1.743973  4e-6
r       1.736278
s       1.730658
t       1.726600
e       1.747920  4e-6
"C'"    1.739810  4e-6
"F'"    1.756603  4e-6
END DATA

begin nominal
1.5296  1.71824
1.060   1.72565
end nominal
```

Figure 16 Example Input file for MELT (*Sample 1*)

entered with the *MODEL* command. Commands in the sample-specific file, or entered from the keyboard, will supersede commands in this setup file. Command entry from the keyboard is accepted after both the setup file and the sample-specific file are read.

```
! MELT.MEL

! Setup file for MELT.EXE

BEGIN FORMULAS

! The following lists the formulas which are coded into the program.  Token #1
! is the model number that is selected with the MODEL keyword.  The remainder
! of the line is token #2.  WARNING: do not change the value of token #1 for a
! model since the program is not compiling the following lines.  Changing the
! formula will have no computational effect; changing the model number will
! indicate that an undesired formula has been used during computation.

!     One-term, one-coefficient models.
26    N  =  N0 + B1

!     Two-term, two-coefficient models.
 1    N  =  N0 + B1 + B2*W
18    N  =  N0 + SQRT( B1 + B2*W )
 2    N  =  N0 + B1 + B2/W
19    N  =  N0 + SQRT( B1 + B2/W )
 3    N  =  N0 + B1 + B2*W^2
20    N  =  N0 + SQRT( B1 + B2*W^2 )
 4    N  =  N0 + B1 + B2/W^2
21    N  =  N0 + SQRT( B1 + B2/W^2 )

!     Two-term, three-coefficient models.
22    N  =  N0 + B1 + B2*W^B3
23    N  =  N0 + SQRT( B1 + B2*W^B3 )
24    N  =  N0 + B1 + B2/W^B3
25    N  =  N0 + SQRT( B1 + B2/W^B3 )

!     Three-term, three-coefficient models.
17    N  =  N0 + B1 + B2*W + B3/W
33    N  =  N0 + SQRT( B1 + B2*W + B3/W )
 5    N  =  N0 + B1 + B2*W + B3*W^2
34    N  =  N0 + SQRT( B1 + B2*W + B3*W^2 )
 6    N  =  N0 + B1 + B2/W + B3/W^2
35    N  =  N0 + SQRT( B1 + B2/W + B3/W^2 )
 7    N  =  N0 + B1 + B2*W^2 + B3*W^4
36    N  =  N0 + SQRT( B1 + B2*W^2 + B3*W^4 )
 8    N  =  N0 + B1 + B2/W^2 + B3/W^4
37    N  =  N0 + SQRT( B1 + B2/W^2 + B3/W^4 )
 9    N  =  N0 + B1 + B2*W^2 + B3/W^2
38    N  =  N0 + SQRT( B1 + B2*W^2 + B3/W^2 )

!     Sellmeier forms; 1- 2- and 3-term, 2- 4- and 6-coefficient.
11    N  =  N0 + SQRT( B2*W^2/(W^2-B1^2) )
12    N  =  N0 + SQRT( B3*W^2/(W^2-B1^2) + B4*W^2/(W^2-B2^2) )
13    N  =  N0 + SQRT( B4*W^2/(W^2-B1^2) + B5*W^2/(W^2-B2^2) + B6*W^2/(W^2-B3^2))

!     Six-term, six coefficient models.
32    N  =  N0 + SQRT( B1 + B2*W^2 + B3/W^2 + B4/W^4 + B5/W^6 + B6/W^8 )
```

Figure 17 MELT.MEL Setup File for MELT, part 1

```
!     Forms not involving a known nominal model, N0.

!     Manufacturers' 6-term, 6-coefficient form.
10    N  =       SQRT( B1 + B2*W^2 + B3/W^2 + B4/W^4 + B5/W^6 + B6/W^8 )

!     Cauchy form.
27    N  =       B1 + B2/W^2 + B3/W^4

!     Conrady form.
28    N  =       B1 + B2/W + B3/W^3.5

!     Hartman 1, 2, and 3 term.
29    N  =       B1/(W-B2)^B3
30    N  =       B1 + B2/(W-B3)^B4
31    N  =       B1 + B2/(W-B4) + B3/(W-B5)

!     Sellmeier forms; 1- 2- and 3-term, 2- 4- and 6-coefficient.
14    N  =  SQRT( 1.0 + B2*W^2/(W^2-B1^2) )
15    N  =  SQRT( 1.0 + B3*W^2/(W^2-B1^2) + B4*W^2/(W^2-B2^2) )
16    N  =  SQRT( 1.0 + B4*W^2/(W^2-B1^2) + B5*W^2/(W^2-B2^2) + B6*W^2/(W^2-B3^2))

END FORMULAS

COMPANY 'MELLES GRIOT - ROCHESTER, NY'
MIN_WVL        .4
MAX_WVL        .7
WAVELENGTH    .6328          ! Always compute index at red HeNe for interferometer.
UNCERTAINTY    .0001         ! Assume refractometry from United Lens.
CATALOG       D:\SCIP\GLASDATA\    ! Files of coefficients for N0.
HISTORY YES                  ! Build a histogram of how frequently a model is "best"...
HISTORY FILE E:\THESIS\MELT\WORK\HISTORY.MEL   ! ...in this file.
DEBUG NO                     ! Imbedded print commands turned on/off.
PLOTTER ON HP7470A           ! No device name given, so will create a .PLT file.
PLOT WAVELENGTH              ! ...rather than FREQUENCY.
PRINTER ON LPT1              ! PRINTER OFF if don't want a copy of what's on screen.
FFEND YES                    ! In a PC environment, end report with a form-feed.

! List of models to try;  enter MODEL 0 from the keyboard to flush the list.
MODEL       1 18 2 19 3 20 4 21
MODEL       24 25 17 33 5 34 6 35 7 36 8 37 9 38 32
MODEL       11 12 13
MFTYPE       4               ! Chi-Square merit function.
CONVERGENCE 1.0E-4           ! Smaller values cause simplex optimization to work harder.
RISK        .010             ! have MELT quote 99.0% confidence intervals.
```

Figure 18 MELT.MEL Setup File for MELT, part 2

• Algorithms

The computational methods used to fit the model to the data were summarized in the Methods Section. Optimizing the fit of the model to the experimental data implies minimizing the merit function. Four different merit functions, Eq. (20) through Eq. (23), are provided [page 20] and are selected using the *MFTYPE* command. Each has advantages in certain situations:

MFTYPE 4 *Chi-square (weighted sum of squared deviations)*: This is the same as *MFTYPE 1*, except that the weighting factors are not relative. Here, the Δn_j values are, as nearly as possible, the

standard deviations of the experimental uncertainty in n.* To the extent that the Δn_j values are normally distributed (Gaussian), and independent, minimizing this merit function will give the maximum likelihood estimates of the coefficients b_1, b_2, ..., $b_{k_{max}}$ of Eq. (23). There is only one "correct" model, and a statistical universe of data sets drawn from it; the probability that this data set could have been drawn from this model, with these coefficients and uncertainties, is maximized by this criterion.

MFTYPE 3 *Weighted maximum deviation*: Minimizing this function is appropriate when the data is known to be "exact" and it is desired to fit an empirical equation for predictive purposes. This can be useful for testing the usefulness of alternative models when nominal data is substituted for experimental data.

MFTYPE 2 *Weighted sum of absolute deviations*: When the data set is suspected of containing *outliers*,** using this merit function will reduce their impact on the resulting solution. This facilitates the identification of the offending point(s). They should then be corrected or removed from the data set and the analysis repeated with a more appropriate *MFTYPE*.

This is a *robust* technique that is meant for cases where the Gaussian distribution is a poor approximation for the probability of occurrence of Δn values.

MFTYPE 1 *Weighted sum of squared deviations*: Most often used when the Δn values are not known (i.e., all weight factors are unity). When they are known, *MFTYPE 4* is equivalent and is able to give additional information regarding the quality of the fit.

---

* That is, they are equal to σ_j, which is to say that 68% of the time, the "true" value of n_j will fall within $\pm \sigma_j$ of the measured value; and 95% of the time, within $\pm 2\sigma_j$; $\pm 3\sigma_j$ 99.7% of the time; and so on.

** The term *outliers* refers to experimental points that have apparent measurement errors that are much larger in magnitude than the other points in the data set (digit transposition errors, wrong spectral line used, etc.). Such points can spoil a least squares fit (*MFTYPE 1* or *MFTYPE 4*), which assumes a Gaussian distribution for Δn, since the probability of occurrence of large errors is so small that the whole curve is distorted to try to bring the outliers, mistakenly, into line (Press, p. 501, reference 56).

The chi-square (χ^2) merit function is generally recommended. The worse the fit, the larger the computed χ^2. The table value of the χ^2 distribution, with $\nu = j_{max} \quad k_{max}$ degrees of freedom, may be consulted to determine how large the computed value of χ^2 may be before it is significant (i.e., not attributable to chance alone). Chi-square interpretation is discussed further on page 65.

The *downhill simplex algorithm* [page 21] is employed to minimize the merit function by the optimum selection of the model's coefficients (b_1, b_2, ..., $b_{k_{max}}$). About 50% of the models which MELT may use are linear in these coefficients; the others are nonlinear.* While it is possible to transform most of the nonlinear models into linear ones with some fairly straight forward variable changes, all the uncertainties would need to be changed to maintain proper weighting.** Using all models directly, without any transformations, is advantageous since it avoids any questions about the weighting and allows the direct comparison of the results of one model with the results another. This strategy is not without drawbacks, however. Appendix 8 [page 108] fully discusses the alternate, matrix approach*** which provides certain statistics that cannot be computed with the simplex algorithm.

• Analysis of Variance

Determining which model to use is no small task. The one chosen may be too complex, not complex enough, or of the wrong form entirely. The easiest way to determine whether or not the model fits the data is to visually examine the plot of residuals. An example has been presented [Figure 14, page 40] for which the model fits the data well; the uppermost plot of residuals appears random, and is of the same

---

* Nonlinear means that at least one of the derivatives of the model, with respect to one of its coefficients ($\partial n/\partial b_k$) depends on at least one of the coefficients (i.e., is not constant).

** If the data was of equal variance in the nonlinear problem, then it is of unequal variance in the linear one and will require weighted least squares.

*** At revision 5.x, MELT does <u>not</u> perform optimization with the matrix approach of Appendix 8.

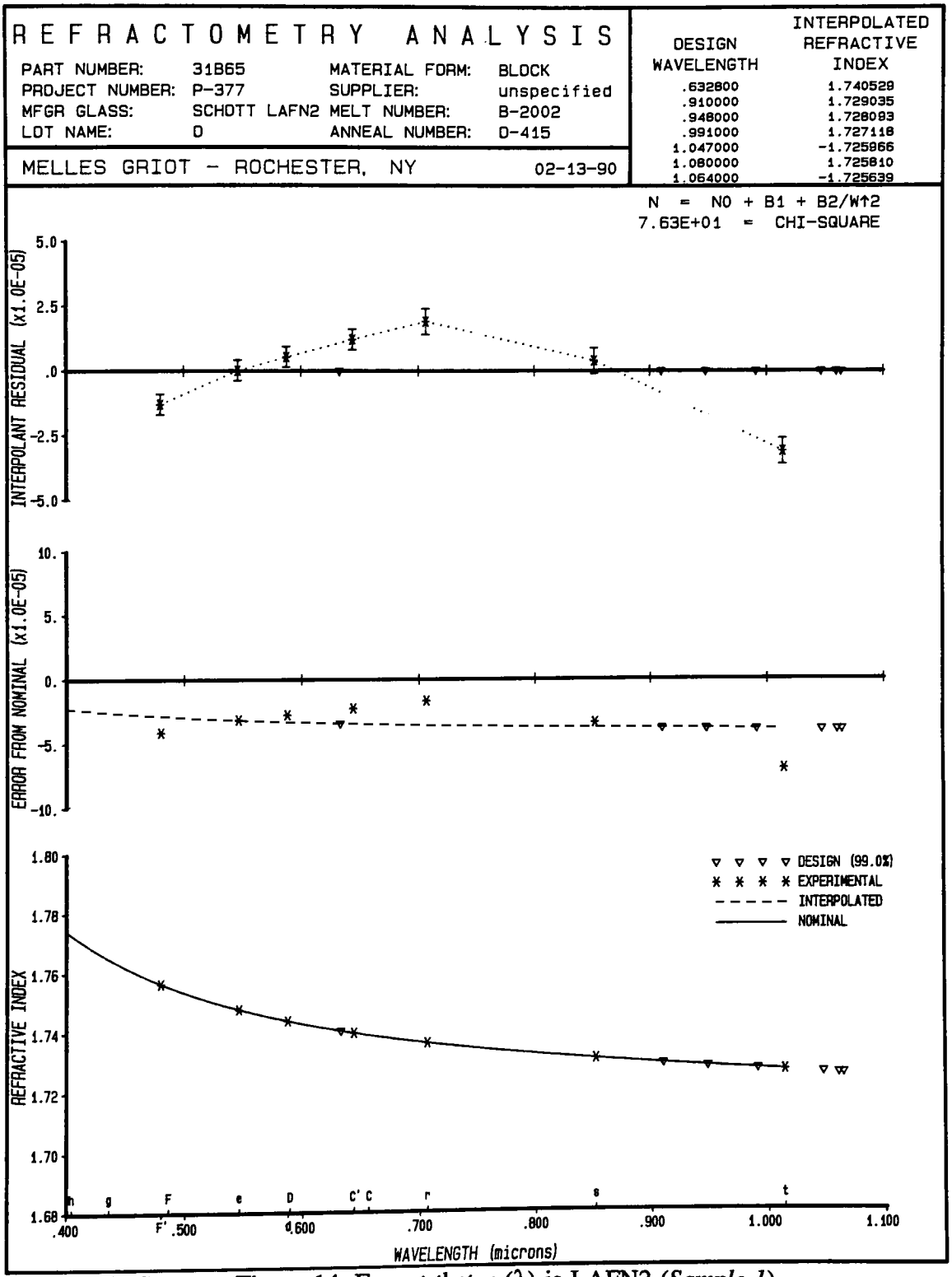

Figure 19 Same as Figure 14, Except that $n_0(\lambda)$ is LAFN2 (*Sample 1*)

order of magnitude as the stated experimental uncertainties in the data set. The model does not fit the same data well in Figure 19. A parabolic trend may be seen in the plot of residuals and is indicative of either a bad $n_0(\lambda)$ for the material under test (via the *GLASS* command), or poorly chosen perturbation terms (via the *MODEL* command). In this particular case, none of the models fit the data, leading to suspicion that the nominal dispersion function, $n_0(\lambda)$, was incorrect for this sample.

A quantitative measure is sometimes needed to describe how well the model fits the data. Visual assessment of "randomness," while convenient, is subjective. Statistical measures are substituted for this visual appraisal whenever fine distinctions are required, or when the assessment must be made by the computer.

Such a situation occurs when MELT is required to choose the best model from a list: what constitutes "best"? Simply choosing the model which results in the smallest merit function value may result in the use of a model having more complexity than the data supports.* To ensure that this does not happen, an analysis of variance (ANOVA) is performed. This analysis must be discussed before the comparison of one model to another.

ANOVA seeks to determine whether or not the model describes, to a significant degree, a real relationship between the variables.** It partitions the variation of the data into categories: the total variation; that explained by a term in the model representing the mean of the data; and that portion of the total variation which is explained by a term, or terms, in the model other than the one that represents the mean. This partitioning is performed in the *sum of squares* space using the following equations:

---

* Simply choosing a model with the same number of coefficients as there are data points will result in a perfect fit (zero residual) which, of course, is a trivial result.

** Unless there are replications (multiple readings of n at the same value of λ) in the data set, ANOVA must stop short of concluding whether any lack of significance is due to measurement errors or to an inappropriate model. See page 62 for a discussion of replicated data.

```
                    A N A L Y S I S    O F    V A R I A N C E

SOURCES                              RELATIVE SS      DF        MS=SS/DF
==============================       ===========      ===       ===========

TOTAL (UNCORRECTED)                     1.000000       7

REGRESSION (DUE TO THE MEAN)             .364335       1      2.11948E-09

TOTAL (CORRECTED FOR THE MEAN)           .635665       6      6.16319E-10

REGRESSION (EXCLUDING THE MEAN)          .631945       1      3.67627E-09

RESIDUAL                                 .003720       5      4.32842E-12


CORRELATION COEFFICIENT
=======================

  DUE TO THE MEAN     =  .3643
  --------------------------
     This implies that approximately  36.43% of the total variation in the
     data is explained by a regression term representing the mean.

  EXCLUDING THE MEAN =  .9941
  ---------------------------
     This implies that approximately  99.41% of the remaining variation in
     the data is explained by regression terms other than the mean.


F-TESTS FOR SIGNIFICANCE OF THE REGRESSION
==========================================

  DUE TO THE MEAN
  ---------------
     F(observed)  =  REGRESSION_MS /  TOTAL_MS     =   3.439

     F(critical)  =  F(  1,  6, .010)              =   13.75

     F(observed)  <  F(critical) implies that a regression term represent-
     ing the mean does not explain a significant amount of the variation
     in the data.  This term should be rejected at this risk level.

  EXCLUDING THE MEAN
  ------------------
     F(observed)  =  REGRESSION_MS / RESIDUAL_MS  =   849.3

     F(critical)  =  F(  1,  5, .010)             =   16.26

     F(observed)  >  F(critical) implies that a significant amount of
     the remaining variation in the data is explained by regression
     terms other than the mean.  These terms should not be rejected.

MFTYPE  Description                                  VALUE
======  ===================================      ==========

     1  WEIGHTED SUM-OF-SQUARED RESIDUALS
     2  WEIGHTED SUM-OF-ABSOLUTE RESIDUALS
     3  WEIGHTED MAXIMUM DEVIATION
 --> 4  CHI-SQUARE                                 1.353


CHI-SQUARE ANALYSIS
===================

Guidelines for CHI-SQUARE:
```

Figure 20 ANOVA for Figure 14 and Figure 15 Data (*Sample 1*)

$$SS_{total} = \sum_{j=0}^{j_{max}} w_j^2 n_j^2 \tag{41}$$

$$SS_{mean} = \sum_{j=1}^{j_{max}} w_j^2 (n_j - \bar{n})^2 \tag{42}$$

$$SS_{corrected} = SS_{total} - SS_{mean} \tag{43}$$

$$SS_{regression} = SS_{corrected} - SS_{residual} \tag{44}$$

$$SS_{residual} = \sum_{j=1}^{j_{max}} w_j^2 \left[n_j - n(\lambda_j;\ b_1, b_2, ..., b_{k_{max}}) \right]^2 \tag{45}$$

Inspection of Eq. (45) will reveal it to be the same as Eq. (20), the weighted sum of squares merit function. Appendix 10 discusses the computation of the average term that appears in Eq. (42). This term may be the simple average, or the weighted average, depending on whether or not the weighting factors differ for any j.

Figure 20 [page 51] shows the ANOVA for the data presented in Figure 14 and Figure 15. In the table at the top of the figure, the column labeled "relative SS" is simply the sum of squares (defined by the five equations above) divided by SS_{total}.* The column labeled "DF" shows the degrees of freedom for each category. The mean

* Actual sum of squares could be determined by simply multiplying MS and DF together.

```
                    A N A L Y S I S    O F    V A R I A N C E

SOURCES                                RELATIVE SS      DF        MS=SS/DF
===============================        ===========     ===     ===========

TOTAL (UNCORRECTED)                       1.000000      8

REGRESSION (DUE TO THE MEAN)               .998597      1     8.66440E-08

TOTAL (CORRECTED FOR THE MEAN)             .001403      7     1.73945E-11

REGRESSION (EXCLUDING THE MEAN)            .001355      5     2.35067E-11

RESIDUAL                                   .000049      2     2.11385E-12


CORRELATION COEFFICIENT
=======================

  DUE TO THE MEAN    =  .9986
  --------------------------
     This implies that approximately  99.86% of the total variation in the
     data is explained by a regression term representing the mean.

  EXCLUDING THE MEAN =  .9653
  --------------------------
     This implies that approximately  96.53% of the remaining variation in
     the data is explained by regression terms other than the mean.


F-TESTS FOR SIGNIFICANCE OF THE REGRESSION
==========================================

  DUE TO THE MEAN
  ---------------
     F(observed)  =  REGRESSION_MS /  TOTAL_MS     =   4981.

     F(critical)  =  F(  1,  7, .010)              =   12.25

     F(observed)  >  F(critical) implies that a significant amount of
     variation in the data is explained by a regression term
     representing the mean.  This term should not be rejected.

  EXCLUDING THE MEAN
  ------------------
     F(observed)  =  REGRESSION_MS / RESIDUAL_MS  =   11.12

     F(critical)  =  F(  5,  2, .010)             =   99.30

     F(observed)  <  F(critical) implies that regression terms other
     than the mean do not explain a significant amount of the
     remaining variation in the data.  These terms should be rejected
     at this risk level.

MFTYPE  Description                                    VALUE
======  ================================          ==========

     1  WEIGHTED SUM-OF-SQUARED RESIDUALS
     2  WEIGHTED SUM-OF-ABSOLUTE RESIDUALS
     3  WEIGHTED MAXIMUM DEVIATION
 --> 4  CHI-SQUARE                                  .1691


CHI-SQUARE ANALYSIS
===================
```

Figure 21 ANOVA for a Model that is too Complex (*Sample 2*)

square column label indicates how "MS" is computed: the sum of squares (not the relative SS) is divided by the degrees of freedom.

In this example, the relative SS due to the term representing the mean is 0.364. This means that 36.4% of the total variation is explained by this term. The relative SS for all remaining terms is 0.632, meaning that they explain 63.2% of the total variation. The *correlation coefficient* (often denoted R^2) says the same thing, but in a slightly different way. It is computed by dividing the regression SS by the preceding total SS. This yields the same result for the regression SS due to the term representing the mean. The correlation coefficient for the terms other than the mean indicates what fraction of the of the remaining variation* is explained by these terms. In this example, R^2 is 0.994 (= 0.632 ÷ 0.636), meaning that 99.4% of the remaining variation in the data set is explained by model terms other than the one that represents the mean.

The sum of squares indicate how much of the total variation in the data is explained by the model, but it is the mean squares that are used to determine if the explained variation is significant. In the limit as the number of degrees of freedom becomes infinite, the mean square becomes the square of the standard deviation; it is called the *variance*, σ^2. The ratio of one variance to another is called an F ratio. This computed ratio is compared to the value of the F distribution to determine if the computed ratio is significant. An example will help to make this clear.

On page 51, in the section of the MELT output labeled "*F* TESTS FOR SIGNIFICANCE OF THE REGRESSION," two F tests are performed. The first determines whether or not the term representing the mean is significant. To do this, the ratio of the variance of the regression due to the mean is divided by the total variance. If the two variances are significantly different from one another, this F ratio will be

* That is, after the term representing the mean has explained some portion of it.

greater than or equal to the *critical value* of the F distribution.* Here, the ratio (3.439) is less than the critical value ($F_{1,6,.01} = 13.75$). The hypothesis, that the term representing the mean is significant, is rejected.

In a similar fashion, the significance of the remaining terms of the regression is tested. Now the question is whether or not the variance of these terms is significantly different from the variance of the residual (i.e., once the terms have explained all of the variation that they can). Continuing with the example of Figure 20, the computed F ratio is much larger (849.3) than the critical value of the F distribution ($F_{1,5,.01} = 16.26$), giving no reason to reject the hypothesis that the terms other than the mean are significant.

The example ANOVA in Figure 21 shows how to detect the usage of a model that is too complex for the data. The F ratio for the term representing the mean (4,981) is larger than the critical value ($F_{1,7,.01} = 12.25$), so it is judged to be significant and is retained. The other terms are not, however. Compare the computed F ratio (11.12) to the critical value ($F_{5,2,.01} = 99.30$). There are five coefficients (degrees of freedom) other than the mean, and two extra degrees of freedom once all coefficients are applied; the greater the number of coefficients, or the fewer the number of extra degrees of freedom, the higher the value of the F distribution—and the more difficult it is to pass the F test.

Figure 22 shows the plotted output from MELT for the ANOVA of Figure 21. Note the high-order behavior in the middle plot in the wavelength neighborhood of 0.4 μm. This type of visual assessment supports the numeric conclusion that the model is more complex than the data will support.

Figure 23 shows the same data fit with the simplest of all models, Eq. (25) [page 25]. The ANOVA gives a clear indication of when the model is too complex,

* The F distribution's value, with the same number of degrees of freedom and *RISK*, is this *critical value*. MELT computes the F distribution's value using an incomplete beta function (Press, p. 169, reference 56). It is denoted as F_0.

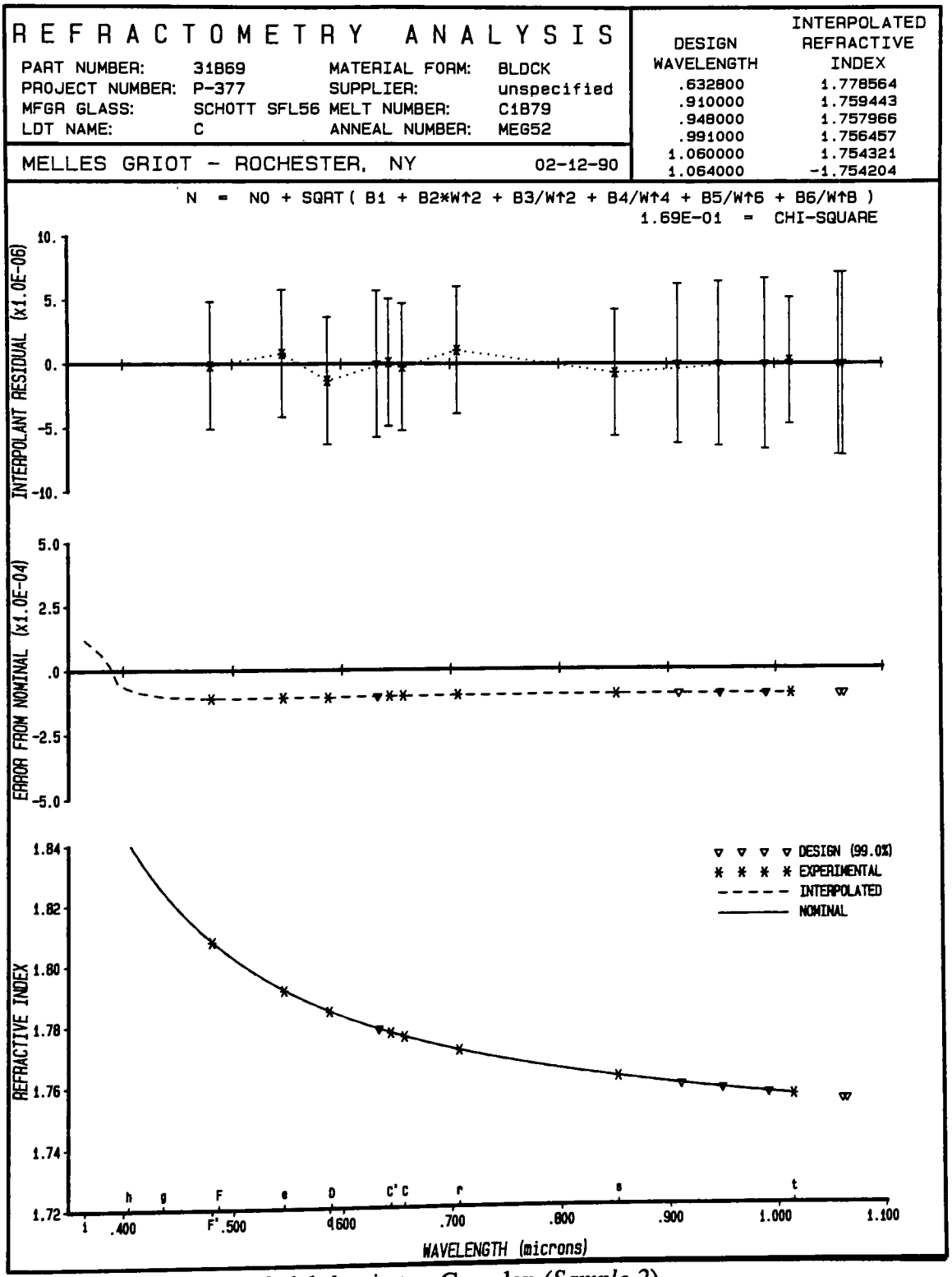

Figure 22 Plot for a Model that is too Complex (*Sample 2*)

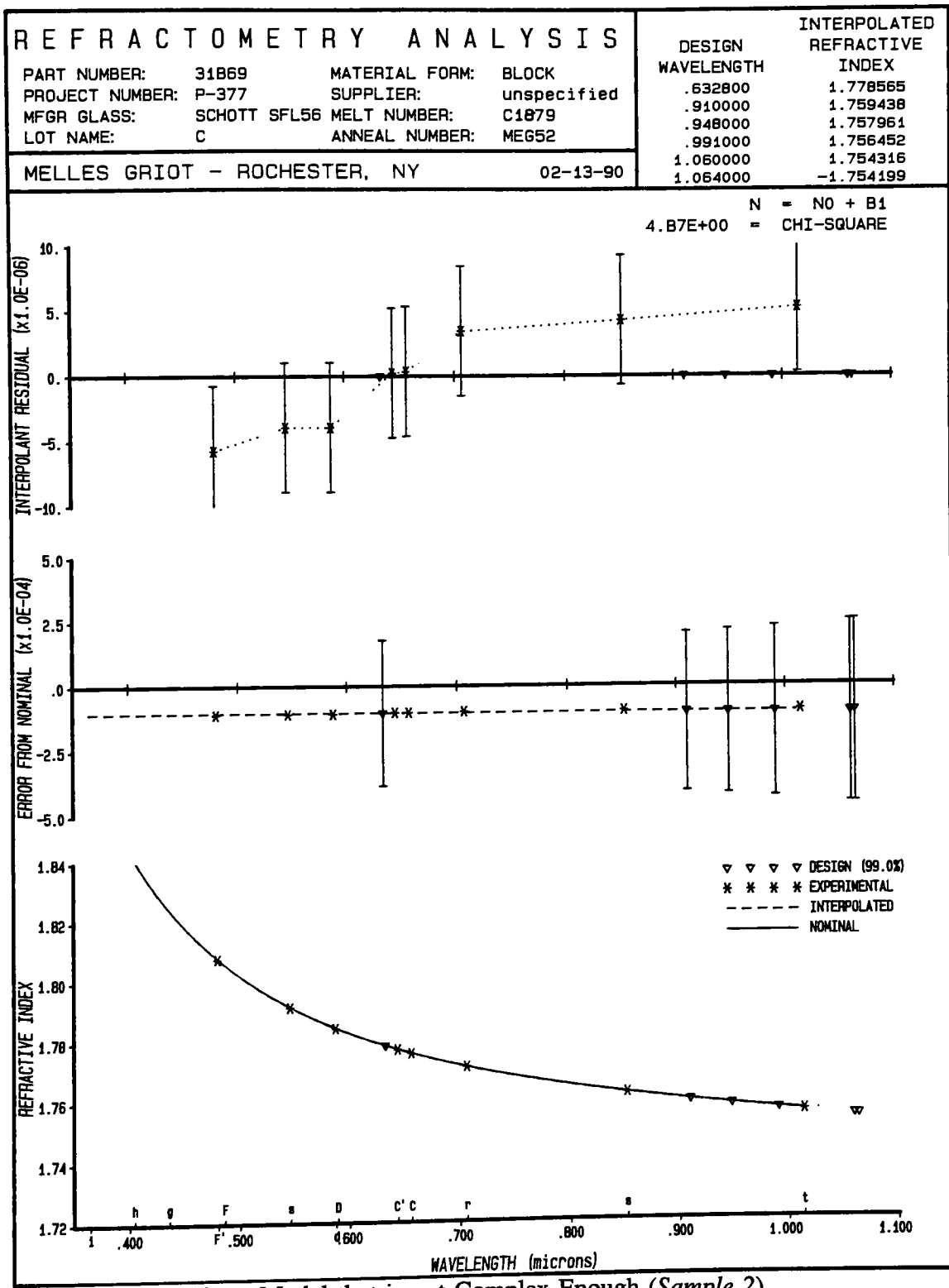

Figure 23 Plot for a Model that is not Complex Enough (*Sample 2*)

but it does not warn that the model is not complex enough.* It is much more difficult to determine the optimum model complexity than it is to ascertain that the model has not become so complex that the data cannot support it.

• Model Assessment

There are two situations that present themselves when assessing the fit and modifying the model. The first is the case where *nested* models are being compared. Non-nested models are compared otherwise. Each demands a different approach.

Nested models are those where the simpler forms are special cases of the most complex form. For example, Eq. (27) is a special case of Eq. (29) [page 25]; furthermore, Eq. (25) is a nested model of both. Nested models are arrived at by zeroing coefficients and allowing terms of the more complex model to vanish. The simplest form that adequately fits the data is desired. Appendix 9 [page 114] describes in detail how nested models are compared using a likelihood ratio test.**

Non-nested models are more troublesome. About all that the field of statistics offers is, "The model resulting in the smallest residual mean square, and the most random-looking residuals, should be chosen."[76] "Random-looking" is a difficult evaluation to accomplish with software like MELT. In Figure 23, the merit function is an order of magnitude worse than in Figure 22 and the residuals now show a trend (and exceed the stated experimental uncertainties). A more complex model is called for, but not as complex as in Figure 22. Just how much more complex is acceptable?***

In the course of performing this research, it was recognized that the quotient of the F ratio (for terms other than the mean) and the critical value of the F distribution

---

* Unless the data has been replicated [see page 62].

** At revision 5.x, MELT does not perform nested model analysis according to Appendix 9.

*** In this particular case, the nested model assessment of Appendix 9 could have been used since the model used for Figure 23 is a special case of the model used for Figure 22—they are not different forms.

(F_0) was always large when a good fit was obtained; when a poor fit resulted, the quotient was not as large. This observation served as the basis of the selection criterion that MELT uses to choose one model from a set of possible models. Figure 24 shows the strategy. When a list of models is supplied to MELT (using one or more *MODEL* commands), the software does a trial solution for each, noting the value of the ratio $F \div F_0$. The model having the highest ratio is selected as being optimum in the sense that it maximizes the margin between the variation that is explained and how much should be explained if it were to be called "significant." After identifying the optimum model, the full analysis is performed.

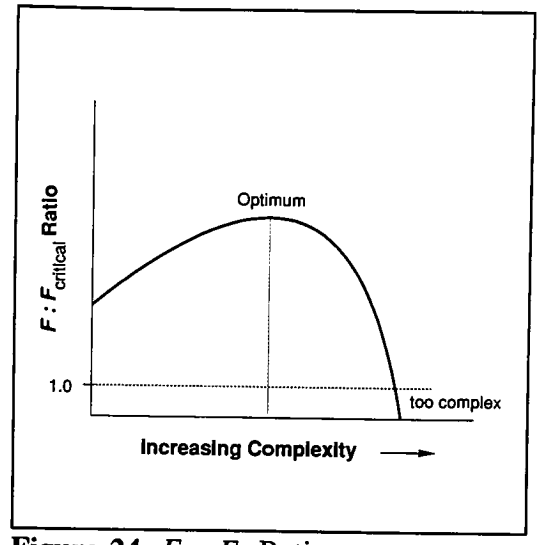

Figure 24 $F \div F_0$ Ratio

In the dialogue shown in Figure 25, MELT is identifying *MODEL 21* as the optimum choice for the sample previously evaluated in Figure 22 and Figure 23; the result is shown in Figure 26.

When no model results in the $F \div F_0$ ratio being greater than unity, then the terms other than the mean are judged to be insignificant for all. In such an instance, MELT will use *MODEL 26* [see Eq. (25), page 25]. This may be indicative of a real manifestation of annealing—simple shifting of $n_0(\lambda)$ in the direction of the ordinate—or it may indicate a data error, or an error in the nominal function, $n_0(\lambda)$. Such a result warrants close examination by the optical designer.

A few nested cases have been compared using this $F \div F_0$ ratio criterion and the maximum likelihood test discussed in Appendix 9. The same model was selected by both approaches. It is not known whether or not the two are generally equivalent for the special case of nested models, or if "cooperative" examples were chosen. The advantage, of course, is that the $F \div F_0$ ratio does not rely on all models being of the same form. The list of models evaluated by MELT in Figure 25 are drawn from 3

```
r       1.771259
s       1.762020
t       1.755710
END DATA

MEL> model        1 18 2 19 3 20 4 21
MEL> model        24 25 17 33 5 34 6 35 7 36 8 37 9 38 32
MEL> model        11 12 13
MEL> go

WARNING   Nominal index computed from the glass table may be in error by more
          than +/-  .000005 for wavelength 1.0640.  The valid range
          is  .3650 to 1.0140.
```

MODEL	ITERATIONS	MERIT	F-TEST FOR TERMS OTHER THAN THE MEAN COMPUTED	CRITICAL	RATIO
1	42	8.39E-01	28.826	13.745	2.10
18	72	8.91E-01	26.813	13.745	1.95
2	42	4.16E-01	64.273	13.745	4.68
19	78	4.28E-01	62.317	13.745	4.53
3	36	1.19E+00	18.469	13.745	1.34
20	65	1.25E+00	17.368	13.745	1.26
4	42	4.24E-01	62.953	13.745	4.58
21	75	4.08E-01	65.610	13.745	4.77
24	129	4.01E-01	27.900	13.274	2.10
25	119	3.98E-01	28.122	13.274	2.12
17	66	3.81E-01	29.480	13.274	2.22
33	106	3.70E-01	30.421	13.274	2.29
5	69	3.01E-01	38.010	13.274	2.86
34	86	8.91E-01	11.172	13.274	.84
6	79	4.04E-01	27.642	13.274	2.08
35	115	4.01E-01	27.884	13.274	2.10
7	101	2.79E-01	41.126	13.274	3.10
36	104	2.84E-01	40.336	13.274	3.04
8	70	3.75E-01	30.002	13.274	2.26
37	112	3.80E-01	29.520	13.274	2.22
9	66	4.20E-01	26.478	13.274	1.99
38	110	4.08E-01	27.338	13.274	2.06
32	348	1.69E-01	11.120	99.299	.11
11	64	4.99E-01	52.619	13.745	3.83
12	90	6.43E-01	8.766	16.694	.53
13	161	4.22E-01	4.212	99.299	.04

```
MODEL 21, using  2 out of  8 degrees-of-freedom, is optimum.

                R E F R A C T O M E T R Y   A N A L Y S I S

PART NUMBER:      31869          MATERIAL FORM: BLOCK          MODEL NUM:    21
PROJECT NUMBER:   P-377          SUPPLIER:      unspecified    MFTYPE NUM:   4
MANUFACTURER:     SCHOTT         MELT NUMBER:   C1879          ITERATIONS:   75
GLASS TYPE:       SFL56          ANNEAL NUMBER: MEG52          MERIT:        4.1E-01
LOT NAME:         C              ANALYSIS DATE: 02-13-90       CONVERGENCE:  1.0E-04
```

Figure 25 MELT Searching for the Optimum Model (*Sample 2*)

broad groups, with many nested forms within each. MELT's criterion appears to be insensitive to changes in the form of the model, making it useful for ranking in non-

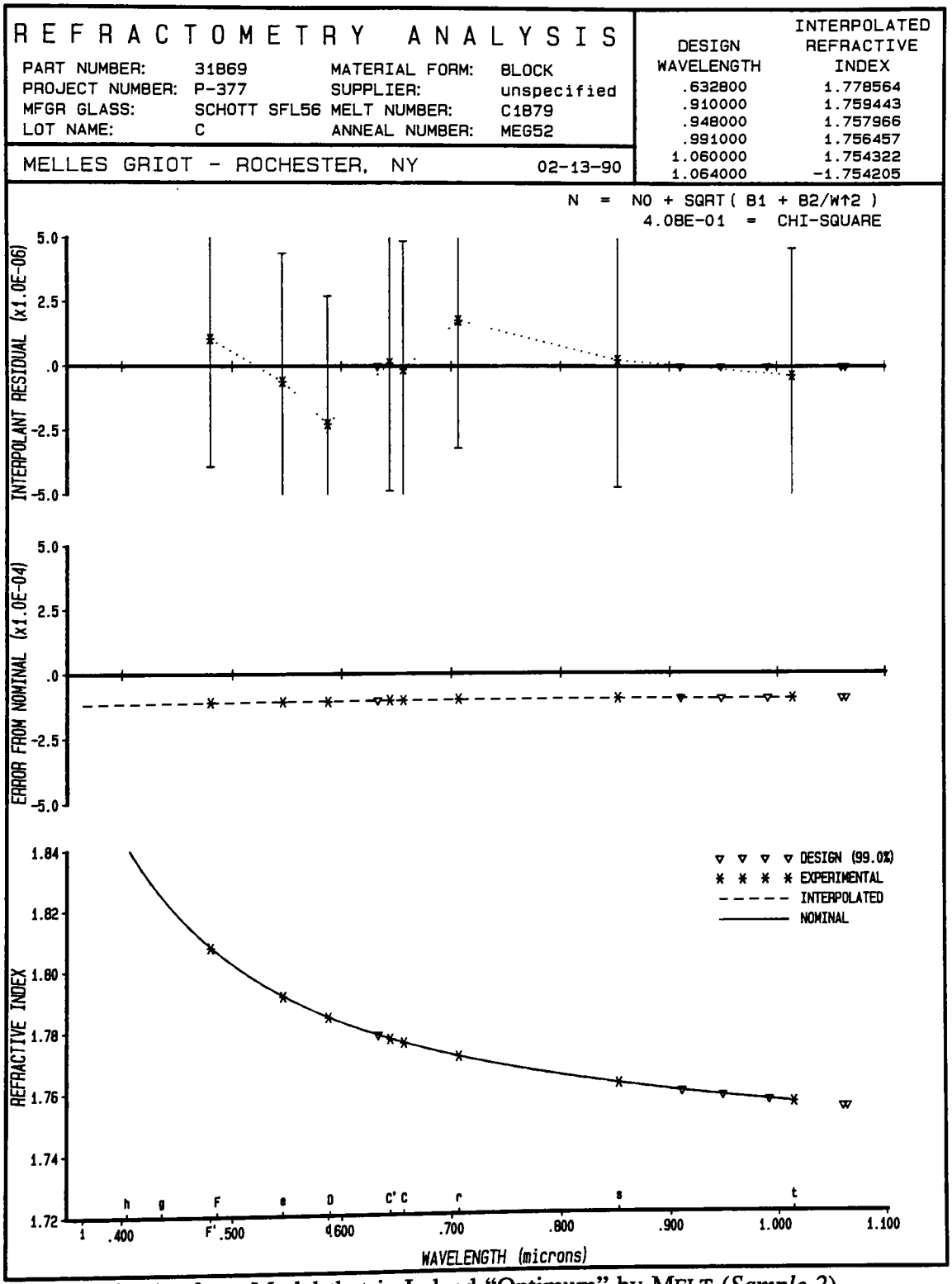

Figure 26 Plot for a Model that is Judged "Optimum" by MELT (*Sample 2*)

nested problems.*

In addition to the possibilities that the model may be too complex, or not complex enough, the model may just be the wrong form. This can be exceedingly difficult to determine if there are not *replications* made of the experimental data points. Replicated data can also help diagnose instances where the model is of insufficient complexity, a situation that ANOVA is unable to detect otherwise.

• Replications

In the ANOVAs presented so far, the SS_{total} is partitioned into categories [page 52], yielding $SS_{residual}$ once the model has been fit to the data. This residual consists of error in the measurements, and lack-of-fit of the model to the data. Only by replicating the data is it possible to further partition $SS_{residual}$ into these two additional categories. In the absence of replications, SS_{error} and SS_{lof} remain *confounded* as $SS_{residual}$. Only subjective tests (trend in the residual?) of model adequacy may be performed if SS_{lof} cannot be separated from SS_{error}.

Replications are multiple readings of n at the same value of λ. These are not simply *duplicate* measurements, where the scale readings are double checked in the course of a single experimental procedure. Instead, replications ideally involve the preparation of two (or more) samples of the same material and repetition of the experimental procedure.** These independent measurements are treated as nearly alike as possible. Any measurement differences that are observed are attributed to chance and untested factors,[77] and collectively referred to as "experimental error." It is not necessary to replicate at each λ in the data set, nor is it necessary that each point be replicated the same number of times.

---

* It is sensitive to a change in the space of the function's range. When some models map to n-space, and others map to n^2-space, the selection criterion has been found to be unreliable.

** Useful information regarding the experimental error inherent in the measurement process is garnered even by repeating the experiment with a single sample, though the influence of sample preparation errors (like curved prism faces, etc.) remain confounded.

Replications do not contribute to expanding the model to cover a larger domain, nor do they reduce the interval between data points. The tendency is to discount their importance and concentrate on taking data at more separate and distinct values of λ, rather than spend precious experimental time repeating measurements at λ values for which data has already been collected. This is misplaced frugality, however, for replications provide increased sensitivity to a poor model without having to increase the inherent precision or accuracy of the experimental equipment. This is numerical leverage!

For j_{max} unique λ_j values, and $i_{j,max}$ replications for each λ_j (each denoted n_{ji}), the partitioning in sum of squares space may be continued from Eq. (45) as follows:

$$SS_{error} = \sum_{j=1}^{j_{max}} \sum_{i=1}^{i_{j,max}} w_{ji}^2 (n_{ji} - \bar{n}_j)^2 \tag{46}$$

$$SS_{lof} = SS_{residual} - SS_{error} \tag{47}$$

As before, Appendix 10 discusses the use of the simple versus weighted average.

An example will help to show the utility of having replications in the data set. Figure 27 shows an ANOVA where the term representing the mean is significant, and the other terms are also significant (see the F tests for significance of the regression); by all indications, the regression is significant and should be accepted. Replicate data allows error to be partitioned from lack-of-fit and, by forming an F ratio of the variance for lack-of-fit to the variance for experimental error, the significance of the lack-of-fit may be judged with respect to the errors in the measurements. Here, the lack-of-fit is found to be significant,* implying that the model should be rejected (even

* The computed F ratio is 15.01 (= $MS_{lof} \div MS_{error}$), which is greater than the critical value ($F_{10,12,.01} = 4.296$) so lack-of-fit is judged "significant" compared to the error.

```
                A N A L Y S I S    O F    V A R I A N C E

SOURCES                              RELATIVE SS      DF        MS=SS/DF
================================     ===========     ===     ===========

TOTAL (UNCORRECTED)                     1.000000      24

REGRESSION (DUE TO THE MEAN)             .637562       1     4.86092E-07

TOTAL (CORRECTED FOR THE MEAN)           .362438      23     1.20144E-08

REGRESSION (EXCLUDING THE MEAN)          .344065       1     2.62323E-07

RESIDUAL                                 .018374      22     6.36757E-10

ERROR                                    .001360      12     8.64340E-11

LACK-OF-FIT                              .017013      10     1.29715E-09


CORRELATION COEFFICIENT
=======================

  DUE TO THE MEAN     =  .6376
  ---------------------------
     This implies that approximately  63.76% of the total variation in the
     data is explained by a regression term representing the mean.

  EXCLUDING THE MEAN =  .9493
  ---------------------------
     This implies that approximately  94.93% of the remaining variation in
     the data is explained by regression terms other than the mean.


F-TESTS FOR SIGNIFICANCE OF THE REGRESSION
==========================================

  DUE TO THE MEAN
  ---------------
     F(observed)  =  REGRESSION_MS /  TOTAL_MS     =   40.46

     F(critical)  =  F(  1, 23, .010)              =   7.881

     F(observed)  >  F(critical) implies that a significant amount of
     variation in the data is explained by a regression term
     representing the mean.  This term should not be rejected.

  EXCLUDING THE MEAN
  ------------------
     F(observed)  =  REGRESSION_MS / RESIDUAL_MS  =   412.0

     F(critical)  =  F(  1, 22, .010)             =   7.945

     F(observed)  >  F(critical) implies that a significant amount of
     the remaining variation in the data is explained by regression
     terms other than the mean.  These terms should not be rejected.


F-TEST FOR SIGNIFICANT LACK-OF-FIT
==================================

     F(observed)  =  LOF_MS / ERROR_MS  =   15.01

     F(critical)  =  F( 10, 12, .010)   =   4.296

     F(observed)  >  F(critical) implies that the lack-of-fit of the
     model to the data is significant compared to the errors in the
     measurements and that the model should be rejected.
```

Figure 27 ANOVA for a Model which is of the Wrong Form (*Sample 3*)

though the other F tests show that the regression terms are "significant"). Had the data set contained replications which had a greater variance (greater range of values), then the lack-of-fit would have been less significant compared to these larger errors and the chance of model rejection lessened. Experimental precision, not accuracy, allowed the model to be diagnosed as inadequate.

Appendix 11 presents a full MELT analysis involving the same replicated data which was used for Figure 27. *MODEL 4* was used for the analysis presented in Figure 27; MELT identifies *MODEL 24* as optimum in Appendix 11.

• Chi-square

Comparing the value of the chi-square merit function, χ^2, to the value of the χ^2 distribution gives yet another indication of whether the model fits the data. The smaller the χ^2, the better the fit. The probability Q that the observed χ^2 could even be larger than its current value, and still be attributable only to chance (i.e., χ^2 may be larger *even* for the correct model), may be defined[78] as an incomplete gamma function,

$$Q\left(\frac{\nu}{2},\frac{\chi^2}{2}\right) = \frac{\Gamma\left(\frac{\nu}{2},\frac{\chi^2}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)} \quad , \tag{48}$$

where ν is the number of degrees of freedom in the residual, χ^2 is the observed chi-square (merit function value), and Γ is the gamma function. The closer Q is to unity, the more probable that the model is correct.

If Q is very small, then the errors are unlikely to be due to chance. It is more likely that the model is wrong, or the stated experimental uncertainties are underestimated—they should really be larger. Truly wrong models will often result in

$Q << 10^{-3}$; it is reasonable for real-world experimental data, using the correct model, to result in $Q \geq 10^{-1}$; $Q \approx 1.0$ is an indication that the stated experimental uncertainties are overestimated—they should be smaller—or possibly that the data is not the result of experiment.[79] An example chi-square analysis, for the data presented in Figure 27, may be found on page 123 in Appendix 11.

As the number of degrees of freedom ν becomes large, the χ^2 distribution becomes normally distributed with a mean of ν. This suggests a goal of $\chi^2 \approx \nu$. If the computed value of χ^2 is smaller than ν, the stated experimental uncertainties may be too large (i.e., too conservative); too large a value of chi-square may simply indicate a poor fit, or that the stated Δn_j values are too small. When the other goodness-of-fit measures are used, comparing χ^2 to ν is an excellent way to refine the estimates of the experimental uncertainties, Δn_j.

• Results

The null hypothesis [Figure 3, page 15] has been tested by watching for significantly different "Error From Nominal" plots* when samples of the same melt, but different annealings, are encountered. "Significant" means that the curve shapes are different. Simple vertical displacements from one another are insignificant; H_0 assumes such an occurrence to be an expected result of annealing differences.

On the next pages, Figure 28 and Figure 29 summarize the characteristics of two annealings of Ohara SFL6 glass.[80] Comparing the middle plots of each Figure reveals that the two curves are displaced from one another, and, more importantly, they are not quite the same shape. To determine if the difference in shape is significant the two Figures are shifted vertically, with respect to one another, until the middle plots intersect at λ = 550 nm. The index at λ = 450 nm (n_{450}) would be 0.000053 (± 0.000074) lower for anneal #314 (Figure 29) than for #313; n_{650} would be 0.000030 (± 0.000070) higher for anneal #314 than for #313. These differences are smaller than the ± 95% confidence intervals (shown in parenthesis) so the difference is judged to be insignificant at this risk level.**

Such results do not prove H_0. All that can be said is that they do not disprove it. A single counter example is all that would be necessary to reject H_0 in favor of H_1. Only 3 sets of samples*** have been encountered in 2 years of normal production at our plant with which to test H_0. On the basis of the data collected and reviewed so far, it is not necessary to reject H_0 in favor of H_1. It is possible that a larger sampling would have resulted in a different conclusion.

---

* The middle plot generated by MELT [see Figure 14, page 40].

** The intervals would be even larger if quoted to ± 99% confidence. MELT output that accompanies the summaries presented in Figure 28 and Figure 29 may be found in Appendix 12.

*** The two Ohara SFL6 examples shown here were drawn from a set of 15 different annealings of the same melt. Other sets involving Ohara SFL03, and Schott ZKN7 were also evaluated. The latter sets showed less variation between annealings than the example presented here.

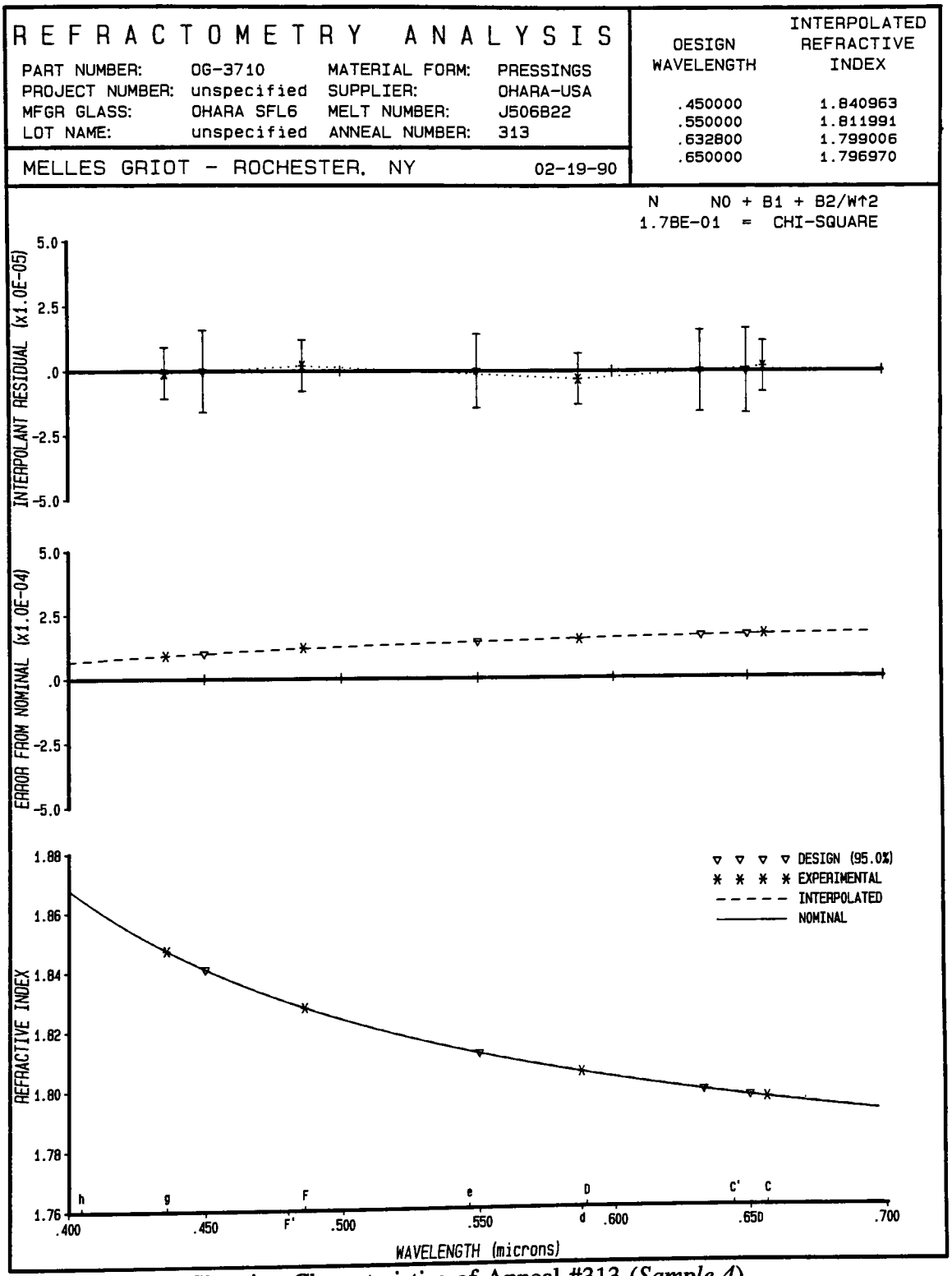

Figure 28 Plot Showing Characteristics of Anneal #313 (*Sample 4*)

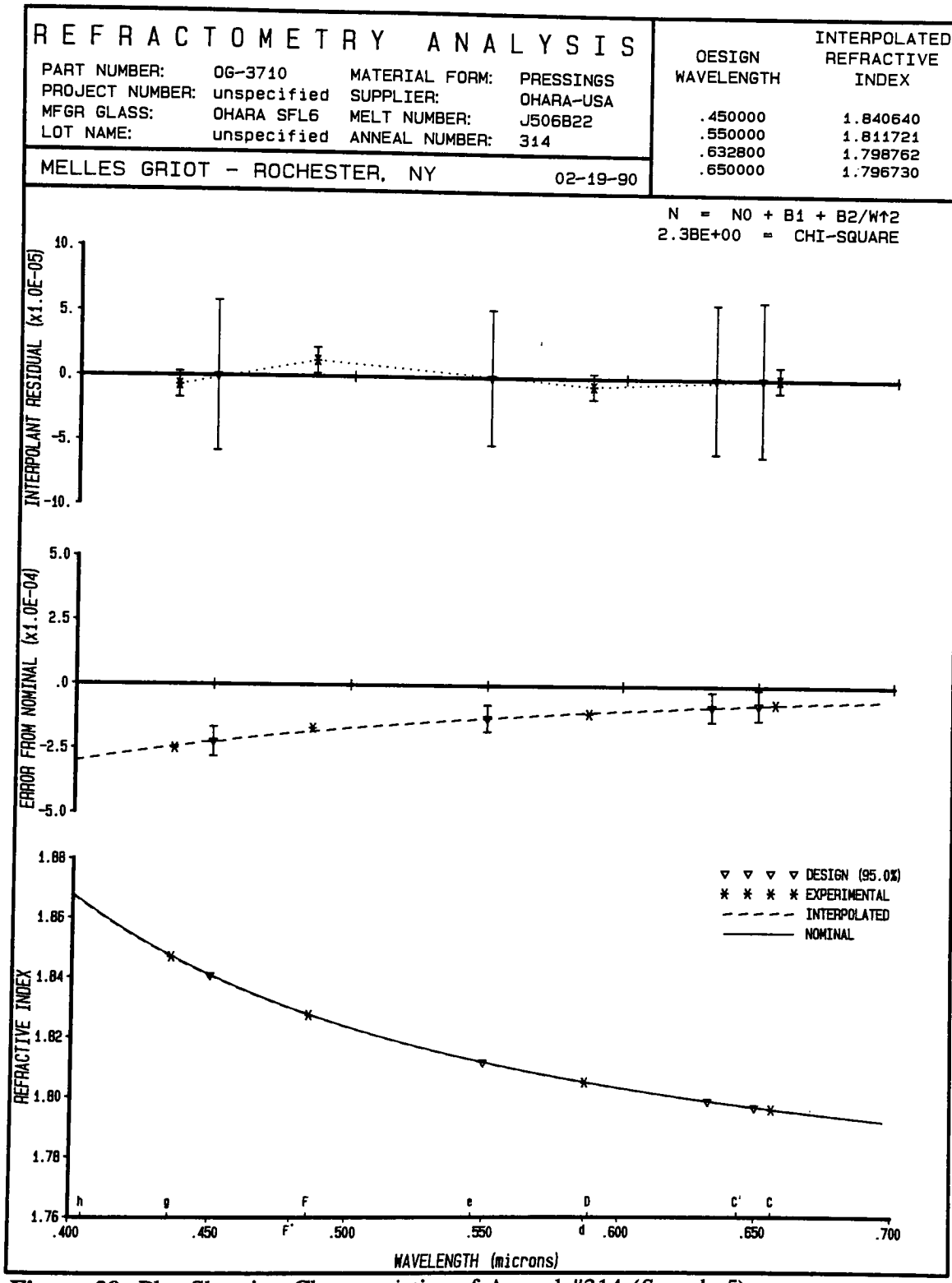

Figure 29 Plot Showing Characteristics of Anneal #314 (*Sample 5*)

Approximately 200 samples have been analyzed by MELT in the two years that it has been in use. From this broad sampling of many glass types and melts, it is possible to report which interpolation models are used most frequently. This information can be used to restrict the search list (MELT's *MODEL* command), or as a starting point in hand calculations.

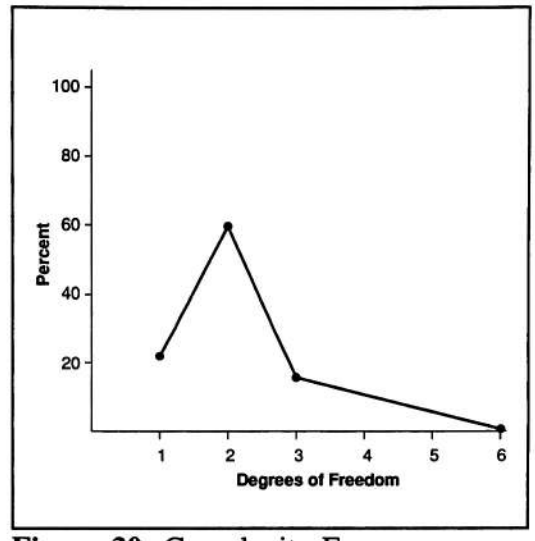

Figure 30 Complexity Frequency

The confidence level (MELT's *RISK* command) impacts how often a model is judged to be "best." Figure 7 [page 26] shows the relative frequency that models are identified by MELT as being optimum at a 95% confidence level (*RISK .05*); Figure 31 shows the same study conducted at the 99% confidence level. As the confidence of our conclusions is raised, the complexity of the model that can be defended

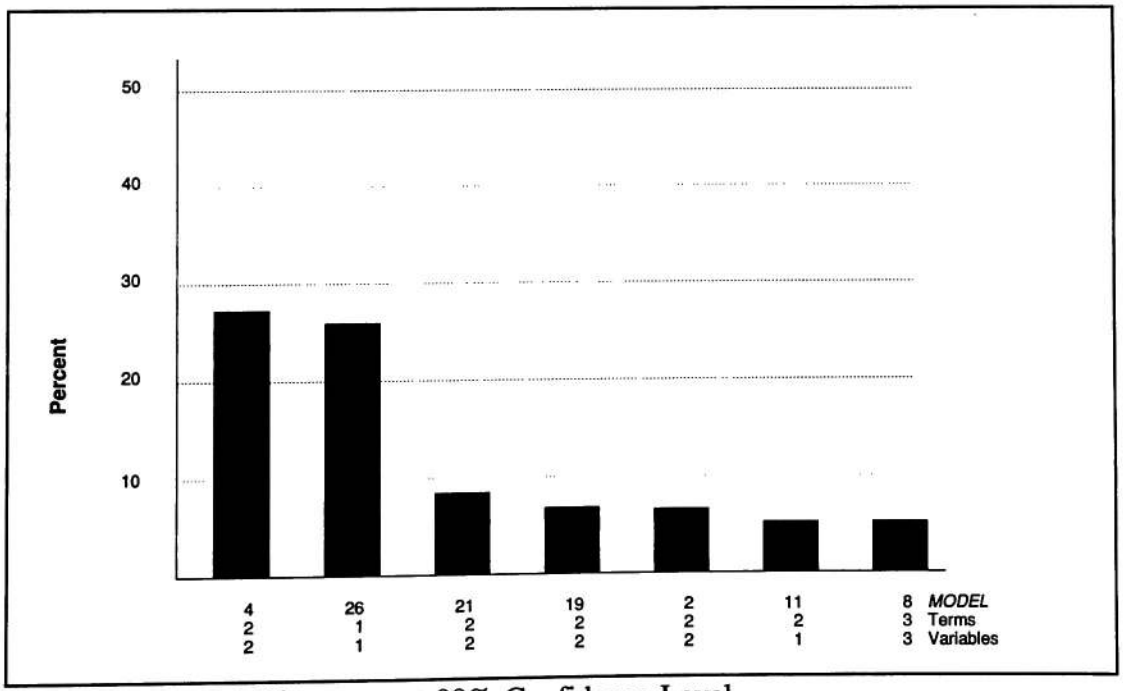

Figure 31 Model Histogram at 99% Confidence Level

is lowered. Figure 30 summarizes the frequency that models having 1, 2 and 3 degrees of freedom are identified as optimum, with the confidence level as a parameter. As 100% confidence in our conclusion is approached, the use of the simplest perturbation model [Eq. (25), page 25] becomes more and more likely. Models with 3 or more degrees of freedom become less probable. Those with 2 occur most often, and 60% of the time—regardless of the confidence level. *MODEL 4* is the most frequently occurring model having two degrees of freedom [Eq. (27), page 25].

V. Conclusions

• Annealing Effect on Dispersion

The observed variation of dispersion, from one annealing to another of samples from the same melt, is insignificant compared to the experimental errors in the measurements. No reason has been found to believe that different annealings of the same melt may have different partial dispersion properties. The principal annealing effect has been observed to be a simple shift of the $n(\lambda)$ curve in the direction of the ordinate, n. Different partial dispersions have been observed from one melt to another of the same glass type, however.

• Interpolation Model

When fitting an equation to experimentally determined refractive index data, optimum results are most often obtained by using a model that has only two degrees of freedom. When an interpolation model of this complexity does not fit the data well, it is most likely that a simpler model will be optimum—a single term representing a shift of the nominal curve. A more complex model is sometimes required, but rarely are more than three degrees of freedom warranted. This is a fundamentally different approach than is often taken. Fitting a general dispersion model, with up to six degrees of freedom, can seldom be defended on the basis of test statistics when the glass type under test has an expected "nominal" dispersion function.

• Suggestions for Further Work

Refractive index data should be reported at standard conditions of temperature, pressure, and humidity. If the experiment cannot be performed under these conditions, then the data should be corrected to report what would have occurred had standard environmental conditions prevailed. Of the three, temperature is the most important. Depending on the glass type, the wavelength, and the magnitude of the temperature, Δn due to temperature change ranges from -0.000007/°C (FK51) to +0.000017/°C

(SF11 and SF6) in the vicinity of 20°C. If the laboratory varies by ± 5°C, this can obviously be a problem for *5th* place refractometry. Not only is the absolute magnitude of the data compromised, but so too is the partial dispersion since the temperature coefficients are functions of wavelength. MELT should be modified to take these temperature coefficients of refractive index into account.*

Implementation of the more conventional matrix approach, described in Appendix 8, would be advantageous for a couple reasons. For models that can be linearized by a simple squaring variable transformation, multiple linear regression can yield estimates of the standard errors of the model coefficients. The simplex algorithm is not able to provide such estimates. Since all the dependent variable data is nearly the same magnitude, this transformation would not have impacted the weighting too severely. If the standard errors were made available, coefficients that do not significantly impact the solution could be more easily spotted, making model assessment and modification simpler to perform.

Even if the model were not easily linearized, the matrix approach could still be used to generate starting points for final coefficient optimization by the simplex method. As with all nonlinear algorithms, starting "guesses" for the unknown coefficients are necessary. This is a difficult problem, generally, and can impact the solution that is obtained if local extremes exist in the multidimensional space that the merit function defines.

Finally, if the matrix algorithm were implemented in MELT to augment the simplex routine, it would be possible to examine a greater number of models by using the nested model assessment of Appendix 9. A model with six degrees of freedom has 63 unique combinations of terms. It is not feasible to perform trial solutions for all of them in a production environment where decisions must be made quickly.

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* This is more an effort of software development than research, requiring access to data files containing the $\partial n/\partial T$ coefficients for every glass type from every manufacturer. Optical Research Associates (Pasadena, CA) will be contacted to determine if MELT can gain access to the binary data files that have been built for their CODE V™ optical design software.

VI. Appendices

• Appendix 1: Principal Dispersion Invariance with Annealing

Principal dispersion is the quantity n_F-n_C. When the Abbe number, V_d [Eq. (16)], changes due to annealing the following example shows that the change is due to a change in the quantity n_d-1, not the quantity n_F-n_C:

For Schott LAK-N16 annealed 1°C per hour:[81]

Δn_d	= -.001400	(which is -0.08% of nominal)
ΔV_d	= -.10	(which is -0.2% of nominal)
$\Delta(n_d\text{-}1)$	= -.001400	(which is -0.2% of nominal)

therefore,

$$\Delta(n_F\text{-}n_C) = 0.0$$

given that

$$V_d = (n_d\text{-}1)/(n_F\text{-}n_C) \qquad (16)$$

• Appendix 2: Equivalency of Sellmeier & Kettler-Drude Series

Beginning with the Sellmeier series, Eq. (10), a substitution of an identity is made that ultimately leads to the Kettler-Drude series, Eq. (11):

Proof:

Sellmeier

$$n^2 = 1 + \frac{A_1\lambda^2}{\lambda^2-\lambda_1^2} + \cdots + \frac{A_j\lambda^2}{\lambda^2-\lambda_j^2} + \cdots$$

$$= 1 + A_1\left(1 + \frac{\lambda_1^2}{\lambda^2-\lambda_1^2}\right) + \cdots + A_j\left(1 + \frac{\lambda_j^2}{\lambda^2-\lambda_j^2}\right) + \cdots$$

$$= 1 + A_1 + \frac{A_1\lambda_1^2}{\lambda^2-\lambda_1^2} + \cdots + A_j + \frac{A_j\lambda_j^2}{\lambda^2-\lambda_j^2} + \cdots$$

$$= 1 + A_1 + \cdots + A_j + \cdots + \frac{A_1\lambda_1^2}{\lambda^2-\lambda_1^2} + \cdots + \frac{A_j\lambda_j^2}{\lambda^2-\lambda_j^2} + \cdots$$

Kettler-Drude

$$= B_0 + \frac{B_1}{\lambda^2-\lambda_1^2} + \cdots + \frac{B_j}{\lambda^2-\lambda_j^2} + \cdots$$

Since

$$B_0 = 1 + A_1 + A_2 + \cdots + A_j + \cdots, \text{ and}$$
$$B_j = A_j\lambda_j^2 \text{ for } j \neq 0,$$

And

$$\frac{\lambda^2}{\lambda^2-\lambda_k^2} = 1 + \frac{\lambda_k^2}{\lambda^2-\lambda_k^2}$$

• Appendix 3: Gaertner L123 Spectrometer

The instrument shown in Figure 5 [page 16] was acquired by Melles Griot with the help of Mr. Novak. The manufacturer reports that it is approximately 50 years old.[82] It was in good overall condition when aquired, though the divided circle was in poor shape: the scale was so tarnished that it was unreadable. This required immediate attention since the divided circle is of prime importance to any spectrometer.

• Accuracy

The L123 spectrometer utilizes two microscopes to view the divided circle. They are 180° opposed to one another so that errors caused by the residual eccentricity and ellipticity of the divided circle, with respect to the axis of rotation, are eliminated[83] [see page 37].

The divided circle is marked with a division every 10 arc minutes. Each microscope is equipped with a filar eyepiece which further divides the 10 arc minute distance between engravings. There is one division every 1 arc minute in the filar eyepiece. The knob of each eyepiece is also divided, with one scale division every 5 arc seconds. As it is possible to estimate between divisions, the accuracy in determining the spectrometer's rotational setting is at least ± 2.5 arc seconds. Appendix 4 shows that this provides the instrument with the ability to determine refractive index to ± 0.000020 for samples of index 1.5, and ± 0.000031 for samples of index 1.8.

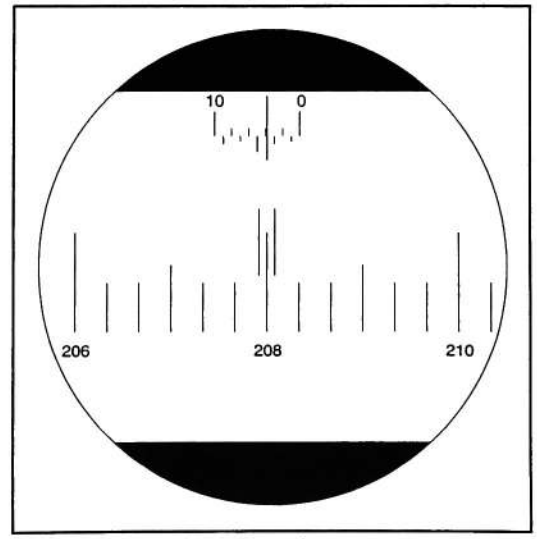


Figure 32 Filar Eyepiece

• Refurbishment

The filar eyepieces were so gummed-up that they were unusable. Both had to be

disassembled and lubricated. Both microscope assemblies required disassembly, cleaning, and magnification adjustment.

The delicate nature of the divided scale complicated the tarnish situation. The scale must be touched to clean it, but to touch it risks damaging it. The 10 arc minute divisions are so lightly engraved that use of even the finest abrasive was out of the question. A metal cleaner by the trade name of "Flitz" was used. It is not abrasive, nor does it have a strong pH. "Birchwood-Casey Blue & Rust Remover", which is a mild solution of phosphoric acid, was used on areas of the scale where a stronger cleaner was required. Great care must be exercised to neutralize the acid solution before the delicate scale divisions are etched away. These operations were performed under a stereo microscope.

• Deficiencies

The L123 is not of an optimal design for refractometry. When measuring D_{min} of a 60° sample, having an index of 1.8, one of the two divided circle microscopes was inaccessible. A right angle viewfinder was adapted to the filar eyepiece to eliminate this flaw.

More serious is the poorly chosen placement of the divided circle. This 170 mm diameter angular scale is attached to the underside of the prism table instead of being buried deep within the instrument's base.* As the prism table is rotated, so does the divided circle. This makes the measurement of D_{min} much more tedious than it would have been had the divided circle remained stationary with prism table rotation. To determine D_{min}, two angular measurements are made: the telescope is swung into position to measure the undeviated ray path, and then into a second position to measure the path of the rays deviated by the refraction of the prism. The angle D_{min} is obtained by subtraction of these two measurements. The design of the L123 makes it

* The design of the instrument allows the operator to touch the delicate scale during routine operation. A protective cover needs to be fabricated to protect it from soiling by finger prints.

necessary to repeat the measurement of the undeviated ray path for every λ since the prism table must be rotated to a different position. If the divided circle were not attached to the prism table, a single measurement of the undeviated ray path could be made and used for all λ. This flaw seriously impacts the operating cost in a commercial setting.

Longhurst[84] and Tilton recommend measuring $2D_{min}$ by setting up the minimum deviation condition twice. The sample is placed on the prism table so that the spectrometer's axis intersects its center. After measuring the path of the rays deviated refraction, the prism table is rotated so that rays from the collimator are incident on the other face. The measurement is repeated; subtraction of the two yields twice the minimum deviation angle, $2D_{min}$. No direct measurement of the undeviated ray path is made. Further, two regions of the divided scale are used, and the orientation of the sample for minimum deviation is repeated. These practices increase the precision of the resulting data.

It is not possible to measure $2D_{min}$ with the L123 since the divided scale is attached to the bottom of the prism table. The more direct approach of measuring the deviated and undeviated ray paths must be exercised. The same number of scale readings must be made using either method, but the latter only involves setting the prism up once for minimum deviation.

The Gauss eyepiece on the observation telescope was inadequate for autocollimation off the prism faces (to determine α). An Abbe-Lamont autocollimating eyepiece is used instead.[85] It has two reticle lines that intersect at 30° in the center of the field of view. An object is introduced from slightly off-axis; the return image will also be slightly off-axis, but on the other side of the reticle intersection point. Both may be

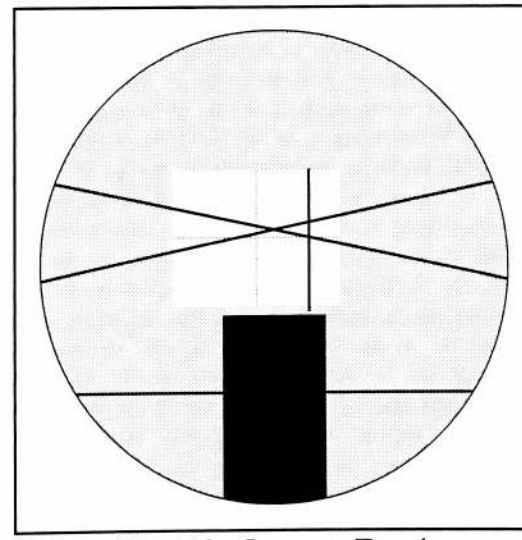


Figure 33 Abbe-Lamont Eyepiece

adjusted to be off-axis by the same amount to high accuracy by rotating the sample or the telescope. The 10x magnification of the eyepiece is barely adequate, however. No higher magnification is available from the manufacturer, and the tube diameter is non-standard making the introduction of a 20-25x eyepiece difficult to accomplish.

• Sources

The visible spectral range is well covered by 3 elements: Cd, He, and Hg. Using only those lines listed below having Fraunhofer designations results in seven data points with approximately 50 nm between each. The full list was used for the example presented in Appendix 11.

Spectral Lines for the Visible Spectrum			
Wavelength	Fraunhofer	Element	Visual Appearance
0.404656 μm	h	Hg	Deep Violet
0.435834 μm	g	Hg	Blue
0.467815 μm		Cd	Blue
0.479991 μm	F'	Cd	Cyan
0.508582 μm		Cd	Green
0.546074 μm	e	Hg	Lime Green
0.576959 μm		Hg	Yellow
0.579065 μm		Hg	Yellow
0.587562 μm	d	He	Orange
0.643847 μm	C'	Cd	Red
0.667815 μm		He	Bright Red
0.706519 μm	r	He	Dim Red

It is difficult to see the h- and r-lines due to the low human visual response at these wavelengths. Caution should be exercised when using the Hg lamp: an ultraviolet cut-off filter must be used to prevent damage to the eye by invisible UV emission.

• Adjustment & Operational Procedure

The following guidelines should be followed when operating the Gaertner L123 as a refractometer:

Eyepiece Focus

Focus the Abbe-Lamont eyepiece on the reticles.

Telescope Focus

Autocollimate off of a prism, or any convenient auxiliary mirror, that is known to be flat to $\lambda/8$ or better, and adjust the focus of the telescope so that the return image of the reticle is sharp.

Collimator Focus

Remove the auxiliary mirror and rotate the telescope so that it views the image of the slit as projected by the collimator. Adjust the collimator focus until the slit image is sharp at the same time that the eyepiece reticle is sharp.

Telescope Perpendicularity with Prism Table Axis

Place a plane parallel piece of glass on the prism table approximately vertical (parallel to the rotation axis of the spectrometer). The reticle image should be visible when autocollimating off of either face of the plane parallel plate.

Adjust the prism table tilt and the tilt of the telescope (perpendicular to the prism table plane) so that the reticle image is the same regardless of prism table rotation. This must be done iteratively. It is not a permanent adjustment and must be repeated periodically. Proceed as follows:

(a) Center the image of the reticle reflected by the first face; (b) Rotate the prism table 180°—the image reflected from the second face will be at a different height in the field; (c) Adjust the prism table leveling screws to reduce the error by 1/2, and then adjust the telescope tilt so that the reticles are now centered; (d) Rotate the prism table another 180° and repeat the procedure until the reticle image remains centered regardless of prism table rotation.

Collimator Axis Parallelism to the Telescope

The height of the collimator, relative to the telescope, is not sensitive. It may be judged visually by sighting along the prism table surface to first the telescope and then the collimator. Adjust the collimator so that it is at the same height as the telescope.

To adjust the collimator's tilt, move the step aperture on the slit assembly to its smallest dimension and make the slit reasonably narrow. Remove the plane parallel plate from the prism table and set the telescope 180° from the collimator.

Adjust the collimator tilt, in the plane perpendicular to the prism table plane, so that the image of the slit is centered in the field of view.

Prism Table Tilt for Sample Prism

The two polished faces need to be parallel to the spectrometer's rotation axis. If the base of the prism is not precisely perpendicular to the polished faces, the prism table must be tilted to compensate.

Wax the prism sample to the prism table so that one face approximately intersects the rotation axis and so that the faces are perpendicular to a line drawn between the prism table adjustment screws. In the diagram to the right, line AC intersects XY at a right angle, as does BC intersect XZ perpendicularly. Faces AC and BC are polished; AB is fine ground.

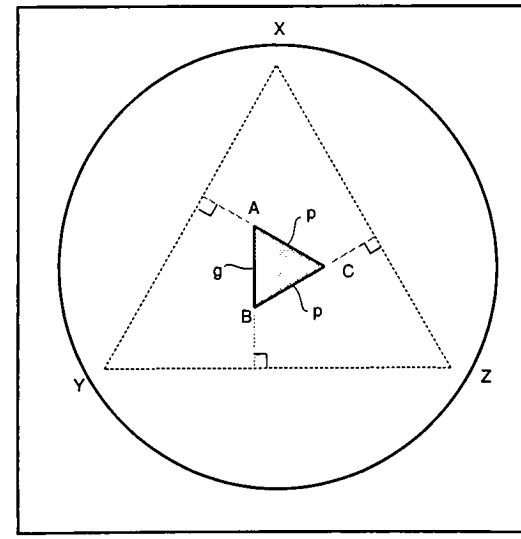


Figure 34 Sample Adjustment

Rotate the prism table, or the telescope, to autocollimate off of face AC and use the prism table adjustment screw at X (or Y) to adjust the tilt of the prism so that the reticle is centered.

Rotate to autocollimate off of face BC and use the screw at Z to adjust. Do not use the screw at X. Repeat until the return image remains centered.

The method just described is more linear than an alternate procedure which begins by centering the prism above the rotation axis of the spectrometer. Fewer iterations will be required to converge on a solution for the tilt of the prism table when following this method.

Measurement of the Prism Angle

Autocollimate off of each of the polished faces of the prism sample and record the readings on a data sheet, like the one shown on the next page. The divided circle is examined twice for each prism face, first with the microscope designated as "1", and then with "2". These data are recorded in the boxes of the same name. It is not important that the two readings differ by precisely 180°.

When making measurements of the divided circle with the filar eyepieces, proceed as follows:

> Move the filar eyepiece pointer so that it is superimposed on the zero minute point in the visual field. Read the pointer on the knob (it probably will not read zero seconds); note where zero is. If the knob is pointed to 20 seconds, then the 25 second point on the knob would be 5 seconds; 15 would be 55 seconds from the previous arc minute. This practice is necessary in order to resolve any ambiguity that arises when taking data since it is often difficult to assess whether or not the pointer is before the minute mark or after. When close to the minute mark, the knob graduations must be consulted to know for certain what the minute reading is. Errors in the data of one arc minute are easily made if this procedure is not followed.

Use the HP-41C program ATON [Appendix 6, page 92] to fill-in the data sheet boxes labeled "AVG" (average). After both scale readings for the second face have been input, "DIF" (difference) is also displayed. It is convenient to write the quantity θ_1-θ_2-180 in the empty space between the boxes labeled "1" and "2" (this quantity should be nearly the same for all measurements if no scale reading errors have been made). Press the A-key to save the angle (displayed as "DIF") as the prism angle, α.

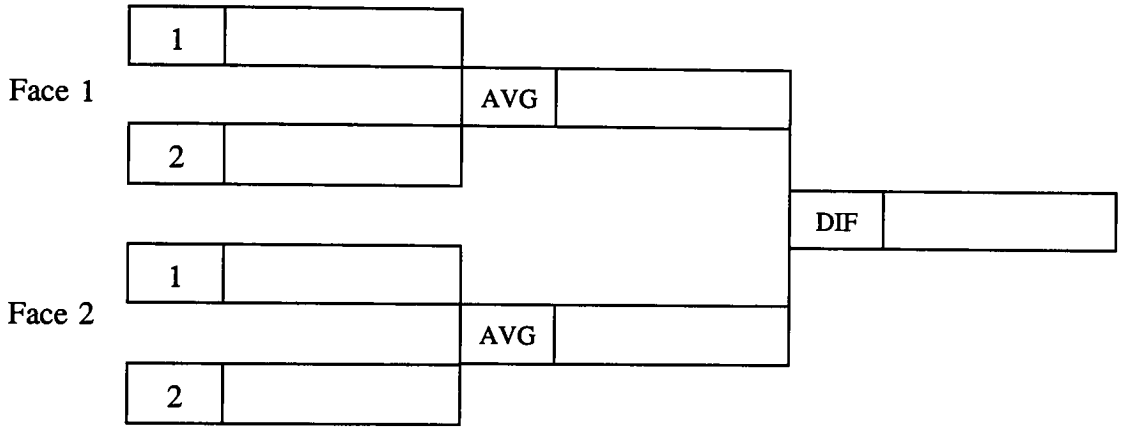
Refractometry Data

Date: _____ Glass: _____ Lot: _____

Part Num: _____ Melt: _____

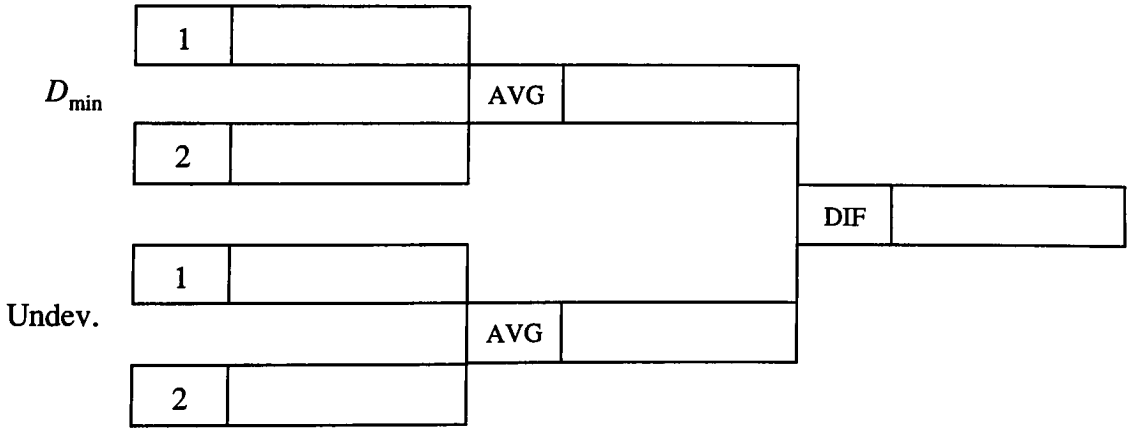
Anneal: _____

Prism Angle



Spectral Data

λ: _____



Computed *n*: _____ - Expected *n*: _____ = δ*n*: _____

Data reduction with the HP-41C program should not be postponed. It is best to compute all angles as the experiment is performed so that potential scale reading errors may be spotted and corrected.

It is also good practice to repeat this measurement, at the conclusion of the session, to further refine the estimate of α.* Appendix 4 [page 85] shows that uncertainty in α has a much greater impact on the computed index than uncertainty in D_{min}.

Measurement of the Minimum Deviation Angle

Install the desired spectral lamp and rotate the prism and observation telescope into positions for minimum deviation refraction through the sample. Following refraction, the source spectra will be dispersed into separate lines. Identify the line of interest.

While watching the image of the slit with the telescope, use the tangent screw adjustment on the prism table and rotate the prism table to the position where the image of the slit slows down, stops, and then goes the other way. This is the minimum deviation position.

Center the reticle of the Abbe-Lamont telescope eyepiece on the slit image. Read the divided scale with the two measurement microscopes and their filar eyepieces. Record the raw scale readings in the boxes labeled "1" and "2", as done for the measurement of α, and then use ATON to compute "AVG" and "DIF". The latter value is D_{min}; press the B-key to save it.

As before, watch for unusual values for the quantity θ_1-θ_2-180. When the same region of the divided scale is continually used, this quantity should remain fairly constant. A large difference from previous values may be indicative of a scale reading error.

Computed Index

All that remains is to press the C-key. ATON will pass to ADN, which will compute n using the spectrometer formula, Eq. (35).

---

* If a better estimate of α becomes available after the raw angular data is reduced to n with ATON, the MELT command *ANGLE* may be used to recompute the experimental values of n based on the new value of α. The values of n are not affected equally by such a change in α.

• Appendix 4: Index Uncertainty due to Angular Uncertainty

Appendix 3 indicates that the Gaertner L123 is able to measure angles to ± 2.5 arc seconds. The prism angle α is the difference of two such readings, so the uncertainty in α is ± 5.0 arc seconds. Two readings are also made and subtracted for D_{min}; it has an uncertainty of ± 5.0 arc seconds as well.

It is presently of interest to determine how this angular uncertainty propagates into uncertainty in the computed index *n*. For *5th* place refractometry, the main contributions are:

- uncertainty in the prism angle α due to goniometric limitations;
- uncertainty in the prism angle due to prism face curvature (Appendix 5 discusses localized changes in α, and how prism placement on the spectrometer's prism table changes the effect on computed index);
- uncertainty in the measurement of the angle of minimum deviation, D_{min}.

Error Propagation of Angular Measurement Uncertainty into Δn						
Sample index, *n*	1.4	1.5	1.6	1.7	1.8	1.9
Prism Angle, α	71°	67°	64°	61°	58°	56°
Min. Deviation, D_{min}	37°46'37.6"	44°46'6.1"	51°57'42.0"	58°16'6.0"	63°32'16.2"	70°15'1.0"
Δn for $\Delta\alpha$ of ± 5"	±0.000012	±0.000015	±0.000019	±0.000023	±0.000027	±0.000032
Δn for ΔD_{min} of ± 5"	±0.000012	±0.000012	±0.000012	±0.000012	±0.000012	±0.000012
Δn for Prism Face Curvature of $\lambda/4$ (λ = 0.5461 μm) over 20 mm Causing $\Delta\alpha$ (Prism Positioned* to ± 1 mm)	±0.000004	±0.000005	±0.000006	±0.000008	±0.000009	±0.000011
Combined Δn (RSS)	±0.000017	±0.000020	±0.000023	±0.000027	±0.000031	±0.000036

* "Positioned" means that the prism is placed on the prism table such that the same region of each face is used for the measurement of D_{min} as for the measurement of α. For placement errors larger than ± 1.0 mm, Δn may exceed the value shown since $\Delta\alpha$ may be relatively large with the polish specification of $\lambda/4$.

If the polish of the prism faces were allowed to be worse than the $\lambda/4$ value given above, finding a compromise focus position for the telescope to allow the accurate measurement of α by autocollimation could be difficult; one face might be convex, and the other concave. For this reason, the polish specification is held to $\lambda/4$ over 20 mm, and the accuracy with which the prism is centered on the prism table is relaxed. For *5th* place refractometry, positioning is required to only $\pm$ 1 mm rather than $\pm$ 0.1 mm.

While it is possible that all components of Δn could take on their extreme values and add unfavorably to cause a combined Δn equal to the sum of the absolute values of the individual effects, this is not likely to occur. It is more probable that the combined uncertainty will be of a magnitude given by the *root sum of squares* (RSS) combination of all components,[86]

$$\Delta n_{\mathrm{RSS}} = \sqrt{\sum_{k=1}^{k_{\max}} \Delta n_k^2} \quad . \tag{52}$$

• Appendix 5: Sample Curvature Effect on Measured Prism Angle α

The spectrometer projects a collimated image of the slit into the space occupied by the prism sample. In the plane of the refraction, this collimated beam is narrow; in the orthogonal plane, parallel to the spectrometer's rotation axis, the beam is the same width as the collimator output aperture. The beam is narrow in the direction of the refraction since the slit is relatively wide in comparison to the wavelength of the illuminating radiation.

Diffraction of radiation through a slit is described by the well-known equation,[87]

$$I = I_0 \frac{\sin^2\beta}{\beta^2} \quad , \text{ where}$$
$$\beta = \frac{\pi d}{\lambda} \sin\theta \quad . \tag{53}$$

In the far field, the intensity drops to zero for values of β that are integer multiples of π. To capture the central lobe of this pattern, which contains most of the energy, it is necessary that the collimator accept at least $\pm\,\theta_0$, the value of θ to the first zero (where $\beta = \pm\,\pi$). This is not a difficult constraint to meet. Usually, the problem is one of under-filling, rather than over-filling, the aperture of the collimator.

The narrower the slit width d, the larger the angle θ_0. A typical slit width in a spectrometer is 150 μm. At a wavelength of 0.5461 μm, θ_0 would be 12.5 minutes of arc (f/135).* This under-fills an f/10 collimator severely. If it has a 25.4 mm output aperture, the collimated beam dimensions in prism-space will be 25.4 mm x 1.8 mm. The limited size of the beam in the direction of refraction will make the computed value of n vulnerable to localized differences in the prism angle α. It is very important that the same region of the faces be used during the determination of D_{min} as was used in the measurement of the prism angle α.

---

* As a rule-of-thumb, the f/number that the central lobe is diffracted into is approximately equal to the slit width in microns (when $\lambda \approx 0.500$ μm).

Prism sample face curvature can give rise to a localized change in the prism angle, as exaggerated in Figure 35; α_2 is not the same as α_1. This change in angle, $\Delta\alpha$, may be quantified in terms of the face curvature.

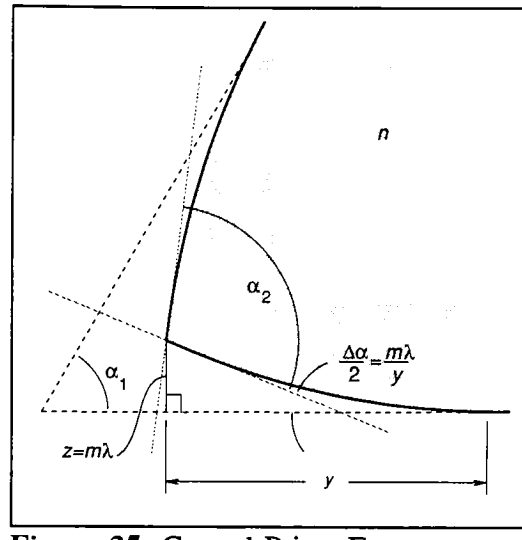


Figure 35 Curved Prism Faces

To the optician, spherical departure from flatness is best expressed in terms of the sagittal distance z from a tangent plane to the surface. This distance z is most often expressed in units of wavelengths, and is called the "sag" of the surface. It may be computed as[88]

$$z = r \pm \text{sign}(r)\sqrt{r^2 - y^2} \quad , \tag{54}$$

though this may numerically fail for $r^2 >> y^2$. Alternatively, with $c = 1/r$, the "-" root may expanded into the series[89]

$$z = \frac{y^2 c^1}{2^1 1!} + \frac{1 y^4 c^3}{2^2 2!} + \frac{1 \cdot 3 y^6 c^5}{2^3 3!} + \frac{1 \cdot 3 \cdot 5 y^8 c^7}{2^4 4!} + \cdots \tag{55}$$

which, in the limit as y or c approach zero, reduces to simply

$$z = \frac{y^2 c}{2} \quad . \tag{56}$$

The angle of incidence at a spherical surface, for a ray parallel to the axis of the surface, is given by

$$\sin I = yc \quad . \tag{57}$$

Rearranging Eq. (56) and substituting it in place of *yc* in Eq. (57) yields an expression for the angle of incidence based on the spherical sagittal departure *z* from a plane, a distance *y* from the point of tangency,

$$\sin I = \frac{2z}{y} \quad . \tag{58}$$

Finally, the sine of *I* is equal to *I* itself (units of radians) as $I \rightarrow 0$, reducing the expression to

$$I = \frac{2z}{y} \quad . \tag{59}$$

The sagittal departure *z* is often expressed in units of wavelengths ($z = m\lambda$). For *m* "waves" of departure from a plane, the angle of incidence at a spherical surface is therefore given by

$$I = \frac{2z}{y} = \frac{2m\lambda}{y} \quad . \tag{60}$$

This result is different by a factor of two from that obtained recently by Tentori & Lerma,[90] where they report the localized change in angle of incidence to be

$$I = \frac{z}{y} = \frac{m\lambda}{y} \quad , \tag{61}$$

a consequence of their linear model that uses the slope of a chord between the pole of the sphere, and the point of intersection of the ray with the surface, to approximate the derivitive. The slope of a tangent line to a sphere is fundamentally different from the slope of a chord to the same point, even in the limit as the chord length approaches zero. The chord model under-estimates the slope by a factor of two.

If the prism face is flat to $\lambda/8$ over a 20 mm diameter at 0.5461 μm, this means that the sagittal distance *z* from the tangent plane to the surface is 0.068 μm at *y* of ± 10 mm. Equation (60) reveals that a ± 2.8 arc second change in α should be

expected across the 20 mm diameter.* Larger or smaller values of z would simply scale this value of $\Delta\alpha$: $\lambda/4$ over 20 mm would result in $\Delta\alpha$ of $\pm$ 5.6 arc seconds, for example.

There are two prism faces, not one. If both are slightly convex—$\lambda/8$ over a 20 mm diameter at 0.5461 μm—then $\Delta\alpha$ is twice the value calculated for one surface by eq. (60). If one face is convex and the other is concave, equal magnitudes of departure from flatness will tend to cancel. This difference in surface curvature makes it more difficult to find a single focus setting for the observation telescope with which to autocollimate off the faces, however, so this is no remedy for prism sample face flatness concerns.

A combination of strategies is necessary to overcome the impact of face curvature on the computed index. It is not feasible to polish the faces flat enough that a random placement of the prism sample in the collimator beam will affect n by an insignificant amount. For example, a sample having n of 1.5 and α of 67° that has been polished flat to $\lambda/8$ (λ = 0.5461 μm) over a 10 mm diameter will have a $\Delta\alpha$ of $\pm$ 1 arc minutes from each 20 mm surface. If both faces are convex by this amount, this would mean that α is 67° $\pm$ 2 arc minutes, depending on where the prism is placed on the prism table!** Care must be exercised to avoid using different regions of the prism face for the measurement of α and D_{min}. Careful placement of the sample on the prism table [page 36], to approximately $\pm$ 0.1 mm, is necessary for *6th* place refractometry. Fortunately, $\pm$ 1 mm is sufficient for *5th* place work. This is not a difficult constraint to meet.

For prism samples having n of 1.5 to 1.8, it is recommend that the faces be polished flat to $\lambda/4$ over a 20 mm diameter (λ = 0.5461 μm), and that the samples be

---

* Tentori & Lerma's results would have been $\pm$ 1.4 arc seconds for the same values of λ, z, and y.

** The computed index n is 1.500000 $\pm$ 0.000360, by Eq. (35).

positioned on the spectrometer's prism table so that the same region of the face is used for the measurement of α as for D_{min} to an accuracy of $\pm$ 1 mm [page 85].

• Appendix 6: Data Acquisition Software for HP-41C

This section assumes a familiarity with the 41C, and HP's RPN keyboard logic. The program ATON calls the other two routines, SAD and ADN. To run ATON, simply execute it from the keyboard: *XEQ ATON*. A listing for ATON is shown on page 95.

Angular input, and output, is in "hours, minutes, and seconds" (HMS). The format is "hh.mmsscc," where "hh" is the number of hours (degrees), "mm" is the number of minutes, "ss" the number of seconds, and "cc" the fractional seconds. For example, 61.04593 would represent the angle 61°4'59.3" of arc.*

ATON displays the following prompt above the keys labeled A, B, ... E:

A	**D**	**N?**	**θ1**	**θ2**	Prompt
A	B	C	D	E	Keys: do/save
a	b		d	e	Keys: delete

To compute *n*, the C-key is pressed. Before *n* may be computed, however, the prism angle must be saved by pressing the A-key, and the minimum deviation angle must be saved by pressing the B-key.

The prism angle is computed by keying in the divided scale reading from the first microscope and pressing the D-key, and then keying the scale reading from the second and pressing the E-key. Pressing the D- and E-keys saves the values; when both have been entered, the computation may proceed. "AVG" is displayed for the form shown on page 83.

The process is repeated for the other prism face, keying in the two angles and pressing the D- and E-keys. Now that two sets of readings have been entered, "DIF" is displayed by ATON too. This is the prism angle, α, in HMS notation. Press the A-key to save it.

---

* See the HP-41C manual for more information.

Values that have been saved may be deleted by pressing the second function of the key. For example, to delete an erroneous entry that was just made for θ_1 by pressing the D-key, press the d-key (the "gold" key followed by the D-key).

The same procedure is followed to compute the minimum deviation angle. After entering two sets of readings for θ_1 and θ_2, "DIF" is again displayed. This is D_{min} in HMS notation. Press the B-key to save it.

Now that ATON has saved the value of α and D_{min}, n may be computed by pressing the C-key. This passes control to the program ADN. Pressing R/S at ADN's prompt returns control back to ATON.

ADN is written in the *interchangeable solution* format, where all but one of the parameters is supplied (by keying the value and pressing the key under the prompt) and the missing one is computed. *What if?* questions are easily answered with such a routine. The spectrometer formula is simply rearranged to provide solutions for α and n. Successive approximation is used to solve for D_{min} if it is the missing parameter. ADN is listed on page 96.

The remainder of the routines in this Appendix are subroutines called by ATON and ADN:

SAD	Passed raw scale readings from the two microscopes, and the last average (of the previous readings). Returns the average of the two scale readings (less 180°), and the difference between this average and the last average. All angles are in HMS.
HMS/	Division of angles in HMS.
HMS*	Multiplication of angles in HMS.
TOL	The display format of the calculator is used to determine the tolerance on iterative solutions (to D_{min} in this case). If 6 places after the decimal are displayed, then TOL returns 1×10^{-6}, for example.
OUT	Displays output at the LCD or printer, depending on hardware.

MLSOL — Solution to $f(x) = 0$ by *modified linear interpolation.*[91] The tolerance on the approximation (from a prior call to TOL), two guesses, and the name of the function being solved are passed.

X3 — Linear interpolation is performed. Two points are passed. X3 returns the value of x for which it predicts that y will equal zero.

$CM — Command processor; this routine provides the saving, deleting, and pointer logic for the interchangeable solution class of programs to which ATON and ADN belong. On entry, the prompt and the number of parameters is passed. On return, the tolerance (from a call to TOL), and the pointer to the missing parameter are passed back. *Synthetic* instructions are necessary* to pass the subroutine return stack around the keyboard input.[92]

* "Synthetic" refers to the fact that the HP-41C's keyboard logic will prevent the entry of some of the instructions used in this subroutine (such as "*RCL [*" and "*STO b*"). Synthetic instructions are used to save the return stack from destruction by the keyboard entry of *XEQ A* through *XEQ e*. This allows control to be passed back to the caller following this keyboard intervention, which is normally impossible.

```
01♦LBL "ATOH"
02 CLX
03 STO 06
04 STO 07
05 X<>F
06 SF 07
07 SF 21
08 SF 27
09♦LBL 14
10 FIX 5
11 "A B H? ∠1 ∠2"
12 PROMPT
13 CF 05
14 GTO 12
15♦LBL A
16 STO 00
17 SF 00
18 CF 05
19 GTO 14
20♦LBL a
21 CF 00
22 GTO 14
23♦LBL B
24 STO 01
25 SF 01
26 CF 05
27 GTO 14
28♦LBL b
29 CF 01
30 GTO 14
31♦LBL C
32 FIX 6
33 XEQ "TOL"
34 XEQ "ADN"
35 CF 05
36 SF 21
37 GTO 14
38♦LBL D
39 STO 03
40 SF 03
41 GTO 13
42♦LBL d
43 CF 03
44 GTO 14
45♦LBL E
46 STO 04
47 SF 04
48 GTO 13
49♦LBL e
50 CF 04
```

```
51 GTO 14
52♦LBL 13
53 FC? 03
54 GTO 14
55 FC? 04
56 GTO 14
57 RCL 03
58 RCL 04
59 X>Y?
60 X<>Y
61 HMS-
62 ADV
63 FC? 55
64 CF 21
65 "1-2="
66 ARCL X
67 AVIEW
68 180
69 X<>Y
70 HMS-
71 SF 21
72 "-180="
73 ARCL X
74 AVIEW
75 RCL 05
76 RCL 04
77 RCL 03
78 XEQ "SAD"
79 STO 05
80 "AVG="
81 ARCL X
82 AVIEW
83 FC? 05
84 GTO 13
85 X<>Y
86 "DIF="
87 ARCL X
88 AVIEW
89 GTO 12
90♦LBL 13
91 SF 05
92♦LBL 12
93 CF 03
94 CF 04
95 GTO 14
96 .END.
```

```
01♦LBL "ADN"
02♦LBL 14
03 -2
04 FC? 07
05 GTO 15
06 CHS
07 GTO 12
08♦LBL 15
09 "A  D  N"
10 XEQ "$CM"
11 X<0?
12 GTO 13
13♦LBL 12
14 STO 09
15 GTO IND X
16♦LBL 00
17 RCL 01
18 HR
19 2
20 /
21 ENTER↑
22 SIN
23 RCL 02
24 RCL Z
25 COS
26
27 /
28 ATAN
29 ST+ X
30 HMS
31 GTO 09
32♦LBL 01
33 30
34 ENTER↑
35 75
36 RCL 10
37 "EE"
38 CF 21
39 XEQ "MLSOL"
40 HMS
41 CLD
42 FS? 05
43 SF 21
44 GTO 09
45♦LBL 02
46 XEQ 02
47 GTO 09
48♦LBL "EE"
49 HMS
50 STO 01
```

```
51 XEQ 02
52 RCL 02
53
54 RTN
55♦LBL 02
56 RCL 00
57 RCL 01
58 HMS+
59 HR
60 2
61 /
62 SIN
63 RCL 00
64 HR
65 2
66 /
67 SIN
68 /
69 RTN
70♦LBL 13
71 FS? 07
72 RTN
73 GTO 14
74♦LBL 09
75 ADV
76 STO IND 09
77 .002
78 STO 09
79 "A"
80 XEQ 08
81 "D"
82 XEQ 08
83 "N"
84♦LBL 08
85 FC? IND 09
86 SF 21
87 RCL IND 09
88 XEQ "OUT"
89 ISG 09
90 RTN
91 2
92 GTO 15
93 .END.
```

```
01♦LBL "SAD"
02 HMS+
03 360
04 X>Y?
05 GTO 13
06 2
07 /
08 HMS-
09 GTO 12
10♦LBL 13
11 2
12 /
13 HMS+
14♦LBL 12
15 2
16 XEQ "HMS/"
17 ENTER↑
18 ENTER↑
19 RCL T
20 HMS-
21 X<>Y
22 .END.
```

```
01♦LBL "HMS*"
02 XEQ 01
03 ST* Y
04 GTO 00
05♦LBL "HMS/"
06 XEQ 01
07 ST/ Y
08♦LBL 00
09 HMS
10 X<>Y
11 HMS
12 STO L
13 CLX
14 RCL T
15 RDN
16 X<> L
17 RTN
18♦LBL 01
19 X<>Y
20 HR
21 X<>Y
22 HR
23 END
```

```
01♦LBL "TOL"
02 0
03 X<>F
04 FS? 36
05 SF 03
06 FS? 37
07 SF 02
08 FS? 38
09 SF 01
10 FS? 39
11 SF 00
12 X<>F
13 CHS
14 10↑X
15 END
```

```
01♦LBL "OUT"
02 "⊢="
03 XEQ "FMT"
04 ARCL X
05 AVIEW
06 CF 21
07 FS? 05
08 SF 21
09 END
```

```
01♦LBL "X3"
02 ST- Z
03 X<>Y
04 ST- T
05 X<>Y
06 RDN
07 RDN
08 /
09 *
10
11 END
```

```
01♦LBL "MLSOL"
02 ASTO 11
03 STO 14
04 RDN
05 STO 13
06 X<>Y
07 STO 12
08 XEQ IND 11
09 STO 15
10 STO 16
11 RCL 13
12 XEQ IND 11
13 STO 17
14♦LBL 15
15 RCL 12
16 RCL 16
17 RCL 13
18 RCL 17
19 XEQ "X3"
20 STO 18
21 VIEW X
22 XEQ IND 11
23 STO 19
24 SIGN
25 RCL 16
26 SIGN
27 X≠Y?
28 GTO 14
29 RCL 18
30 STO 12
31 RCL 19
32 STO 16
33 SIGN
34 RCL 15
35 SIGN
36 X≠Y?
37 GTO 13
38 2
39 ST/ 17
40 GTO 13
41♦LBL 14
42 RCL 18
43 STO 13
44 RCL 19
45 STO 17
46 SIGN
47 RCL 15
48 SIGN
49 X≠Y?
50 GTO 13
```

```
51 2
52 ST/ 16
53♦LBL 13
54 RCL 14
55 RCL 19
56 STO 15
57 ABS
58 X>Y?
59 GTO 15
60 RCL 18
61 END
```

```
01♦LBL "$CM"
02 ASTO 10
03 ASHF
04 ASTO 11
05♦LBL 14
06 STO 09
07 X>0?
08 GTO 15
09 CHS
10 STO 09
11 CF 00
12 CF 01
13 CF 02
14 CF 03
15 CF 04
16 CF 05
17 FS? 21
18 SF 05
19♦LBL 15
20 SF 06
21 CF 21
22 CF 22
23 SF 27
24 CLA
```

```
25 ARCL 10
26 ARCL 11
27 AVIEW
28 RCL a
29 STO \
30 RCL b
31 FC?C 06
32 GTO 10
33 STO [
34 CLST
35 STOP
36 -1
37 FS? 05
38 SF 21
39 RTN
40♦LBL a
41 CF 00
42 GTO 11
43♦LBL b
44 CF 01
45 GTO 11
46♦LBL c
47 CF 02
48 GTO 11
49♦LBL d
50 CF 03
51 GTO 11
52♦LBL e
53 CF 04
54 GTO 11
55♦LBL A
56 0
57 GTO 12
58♦LBL B
59 1
60 GTO 12
61♦LBL C
62 2
63 GTO 12
64♦LBL D
65 3
66 GTO 12
67♦LBL E
68 4
69♦LBL 12
70 X<>Y
71 SF IND Y
72 FS?C 22
73 STO IND Y
74♦LBL 11
```

```
75 RCL \
76 STO a
77 RCL [
78 STO b
79♦LBL 10
80 CLST
81 RCL 09
82 1 E3
83 /
84 0
85 ENTER↑
86 1
87 FS? 05
88 SF 21
89♦LBL 09
90 FS? IND Z
91 ST+ Y
92 ISG Z
93 GTO 09
94 CLX
95 RCL 09
96 X≠Y?
97 GTO 15
98 CF 27
99 XEQ "TOL"
100 STO 10
101 RCL 09
102♦LBL 08
103 FC? IND X
104 RTN
105 DSE X
106 GTO 08
107 .END.
```

• Appendix 7: MELT User's Manual

MELT uses data describing the refractive behavior of a sample of optical glass and fits a dispersion curve to it using nonlinear least squares techniques. This dispersion curve is used to estimate the refractive index at the design wavelengths of an optical system.

• Syntax Rules

MELT parses input into "tokens" that are separated by delimiters. Spaces, a tab, comma, or slash may act as a delimiter. There are three types of tokens: text, real, and integer. There are different rules for each.

Any character is valid in a text string. If text strings contain multiple words, the string should be enclosed by quotes (single or double) so that the individual words are not treated as separate and distinct tokens. If the string contains a quote, then the other type of quote character should be used to surround the entire string.

Real-valued tokens (floating-point numbers) may not contain any alphabetic character other than "E" or "D" (for exponential notation, e.g. 1.5e-5). The parser supports double-precision reals, but most are rounded to single-precision after parsing.

Integer tokens are parsed as reals and then truncated to integers.

Comments may be placed anywhere in MELT files by preceding them with the "!" character. All text following this character is ignored by the command parser.

• Files and Locations

MELT.EXE	Executable file. Must either be in the current directory or in the operating system's search path.
MELT.ERR	Text file containing error code message text. Located in current directory.
input.MEL	Sample-specific file of MELT commands [see Figure 16, page 44, for an example]. Created with any text editor. The full path-name (or a simple filename if in the current directory) is the first command line argument.

MELT.MEL — Setup file containing sample-unspecific MELT commands [see Figure 17, page 44]. Located in current directory.

HISTORY.MEL — Text file keeping track of how frequently a particular model is used. Default location is in the current directory. The filename and location may be changed by using the *HISTORY FILE* command.

MELTHIST.TXT — Text file keeping track of what model was used for each "*input*.MEL" file.

SCHOTT.TXT — Text file containing the manufacturer's coefficients A_0, A_1, ..., A_5 in column-oriented Fortran "1A6,F9.7,5E13.7" format. This file is selected by specifying "SCHOTT" with the *MANUFACTURER* command (which is the default if none is specified). The file is located in the directory given by the *CATALOG* command.

OHARA.TXT — Used instead of SCHOTT.TXT if *MANUFACTURER OHARA* is specified.

HOYA.TXT — Used instead of SCHOTT.TXT if *MANUFACTURER HOYA* is specified.

SOVIREL.TXT — Used instead of SCHOTT.TXT if *MANUFACTURER SOVIREL* is specified.

CHANCE.TXT — Used instead of SCHOTT.TXT if *MANUFACTURER CHANCE* is specified.

```
FK1   2.1392463-.9240937E-02 .8744977E-02 .2146362E-03-.1267199E-04 .6815468E-06
FK3   2.1202375-.8686857E-02 .9140119E-02 .1261317E-03-.8296064E-06 .1318057E-06
FK5   2.1887621-.9557201E-02 .8991523E-02 .1456052E-03-.5284307E-05 .3458801E-06
FK51  2.1883307-.5365879E-02 .7743655E-02 .1312934E-03-.7417952E-05 .4581512E-06
FK52  2.1858571-.5201462E-02 .8107489E-02 .1008583E-03-.2224178E-05 .1919751E-06
PK1   2.2347576-.1000305E-01 .1000085E-01 .1306600E-03-.9595815E-06 .1589902E-06
PK2   2.2770533-.1053201E-01 .1018835E-01 .2900156E-03-.1960286E-04 .1096772E-05
PK3   2.2977022-.1033162E-01 .1075724E-01 .2125515E-03-.8919032E-05 .5785433E-06
PK50  2.2856264-.9849920E-02 .9698452E-02 .2447215E-03-.1633386E-04 .9134481E-06
PSK2  2.4266341-.1059363E-01 .1259096E-01 .1740792E-03-.3262254E-06 .1991616E-06
PSK3  2.3768193-.1014651E-01 .1216715E-01 .1191661E-03 .6425063E-05-.1747871E-06
PSK50 2.3946348-.9685159E-02 .1145794E-01 .1763871E-03-.3450799E-05 .2970466E-06
PSK52 2.5342699-.1034237E-01 .1263637E-01 .3821843E-03-.2874234E-04 .1674809E-05
PSK53 2.5852417-.9429095E-02 .1407447E-01 .2792479E-03-.1277922E-04 .9476918E-06
BK1   2.2513742-.9325402E-02 .1053965E-01 .2259537E-03-.1072905E-04 .7283278E-06
BK3   2.2184519-.1053909E-01 .9911570E-02 .1851256E-03-.7018059E-05 .4238569E-06
BK6   2.3125058-.9539879E-02 .1166875E-01 .1559807E-03 .1162364E-05 .1231805E-06
BK7   2.2718929-.1010808E-01 .1059251E-01 .2081697E-03-.7647254E-05 .4924099E-06
UBK7  2.2715621-.9857157E-02 .1080852E-01 .1406815E-03 .1304180E-05 .4861593E-07
BK8   2.2804948-.9419053E-02 .1134989E-01 .5674176E-04 .1214972E-04-.4277148E-06
BK10  2.2177191-.1024866E-01 .9662766E-02 .1678284E-03-.5532868E-05 .3474742E-06
BK13  2.2839390-.1014860E-01 .1118720E-01 .1467032E-03 .1352335E-05 .1131041E-06
```

Figure 36 Partial Listing of SCHOTT.TXT

When the *READ* command is used to insert a file's contents, the current directory is searched. If it is not found, the directory specified with the *CATALOG* command is searched. The file type ".MEL" is assumed if not specified. It is convenient to create files of nominal index data (for λ outside the range of the manufacturers' dispersion formula) in a subdirectory of the *CATALOG* directory. For example, if *CATALOG D:\SCIP\GLASDATA* is specified, the command *READ NOMINAL\LAF2* will insert the file "D:\SCIP\GLASDATA\NOMINAL\LAF2.MEL" at that point, assuming that "LAF2.MEL" does not exist in the current directory.

```
! LAF2.MEL

BEGIN NOMINAL              ! From Schott catalog
  1.5296        1.71824
  1.060         1.72565
END
```

Figure 37 D:\SCIP\GLASDATA\NOMINAL\LAF2.MEL

• Command Syntax

When MELT is invoked, the name of the sample-specific file is given on the command line. See Appendix 11 for a sample MELT analysis.

The minimum abbreviation for each of the following commands is given in capital letters. Values in square brackets are optional. String lengths are given in parenthesis: "text(30)" means a 30-character text string, for example. When multiple arguments of the same type are allowed, as in a list, the maximum number is given in parenthesis: "real(7)" means that seven floating-point numbers may be given with each separated by a delimiter.

Replicated experimental data may be reported, where there are multiple data points which have the same wavelength. The data will be sorted so that all points with the same wavelength are grouped together.

MELT Commands Providing Sample Identification & Description

Nouns	Value	Description and Defaults
PARt_number	text(12)	Part number that will be made from this material (optional).
PROject_number	text(12)	Project number that the part is associated with (optional).
GLAss_name	text(12)	Name of the glass type under test. If the manufacturer's data dispersion formula is used to supply the nominal indices, then *GLASS_NAME* must be specified. Be aware that all glass names must be expressed in 6 characters or less.
MANufacturer	text(12)	Name of the manufacturer: SCHOTT (the default), OHARA, etc. Used to form the filenames SCHOTT.TXT, OHARA.TXT, etc., when the manufacturer's dispersion constants are required to compute the nominal index. Use "SPECIAL" for material like SILICA or DYNASIL.
MFGr	text(12)	Synonym for *MANUFACTURER*.
MELt_number	text(12)	The manufacturer's melt number (optional).
ANNeal_number	text(12)	The manufacturer's or supplier's anneal number (optional).
SUPplier	text(12)	Name of the supplier (optional).
VENdor	text(12)	Synonym for *SUPPLIER*.
MATerial_form	text(12)	Form of the material: BLOCK, PRESSINGS, etc. (optional).
LOT_name	text(12)	The name or number assigned to this lot of glass (optional).
COMpany_name	text(30)	The name of your company (optional).
TEMperature	real	Permits the temperature (°C) at which the data was acquired to be recorded in the file, but no use is made of this information as of revision 5.x of MELT.
PREssure	real	Permits the barometric pressure (mm Hg) at which the data was acquired to be recorded in the file, but no use is made of this information as of revision 5.x of MELT.

MELT Commands Controlling Input and Output

Noun/Verb	Qualifiers			Description and Defaults
CATalog	text(63)			Drive and directory where SCHOTT.TXT, OHARA.TXT, etc., may be found. By default, the current directory is searched if these files are needed.
PLOt	ON	HP7470A HP7475A HP7550A	[device(63)]	Enables plotting and sets the plot routines to output instructions for the specified plotter. The optional device specification allows output to be sent directly to a device port. If omitted, a file of plot commands is created in the same directory as the file "*input*.MEL" with the name base name and different type: "*input*.PLT".
PLOt	OFF			Turns plotting off (the default).

MELT Commands Controlling Input and Output				
Noun/Verb	Qualifiers			Description and Defaults
PLOt	Wvl			Just plot as a function of wavelength (default).
PLOt	Freq			Just plot as a function of frequency.
PLOt	Wvl	Freq		Plot both by wavelength and by frequency.
PRInter	ON	device or pathname		Send a copy of what was sent to the screen to the specified device or file.
PRInter	OFF			No printed output (default).
SHOrt	[Yes]			Omit the chi-square analysis output and list of models from the printed output.
SHOrt	No			Include the full analysis (default).
FFEnd	[Yes]			In a personal computer environment, the printed report should be followed by a form-feed. This is not needed or desired in a VAX/VMS environment.
HIStory	[Yes]			Turn history file updating on.
HIStory	No			Turn history file updating off (default).
HIStory	File	pathname		Change the name or location of the history file (from HISTORY.MEL in the current directory).
BATch	[Yes]			Do not read the keyboard after MELT.MEL and "*input*.MEL" have been read—an implicit *GO*.
BATch	No			Reset to interactive (default).
BATch	Check			Same as *BATCH YES*, except that the computations are skipped—syntax check only.
QUIt				Abort back to the operating system.
END				If in the middle of a loop, the loop is terminated (see *BEGIN DATA* and *END DATA*, etc.). If not in the middle of a loop, then *END* is equivalent to *GO*.
GO				Terminates keyboard entry and begins the computation.
REAd	pathname			Inserts the contents of the specified file as if it had occurred at the point where the *READ* was encountered. Nested *READ* statements are illegal. See page 102.

MELT Commands for Recording Experimental Results			
Noun/Verb	Qualifiers		Description and Defaults
BEGin	[DATa]		Experimental (observed) data follows, one data point per record, until *END*. Recorded in a sample-specific file.
BEGin	NOMinal		Nominal (expected) data follows, one data point per record until END. Usually put in an auxiliary file that is inserted using the *READ* command.
BEGin	FORmulas		Model number to text translation follows, one model per record until *END*. Usually put in MELT.MEL setup file.
BEGin	HIStory		Historical data follows, one model per record until *END*. Usually put in the file HISTORY.MEL, or some other auxiliary file that is specified using the *HISTORY FILE* command.
END	[previous]		Ends the list that was started with the *BEGIN* command. If in the middle of the experimental data list, then *END* is equivalent to *END DATA*; etc. When an *END* is not pending for any list, *END* is equivalent to *GO*.
END	DATa		Explicitly *END*s the DATA list.
END	NOMinal		Explicitly *END*s the NOMINAL list.
END	FORmulas		Explicitly *END*s the FORMULAS list.
END	HIStory		Explicitly *END*s the HISTORY list.
ANGle	old_angle	new_angle	Changes the experimental data due to better information about the prism angle α becoming available. Both "old" and "new" are in HMS notation. For example, 60.26595 means 60°26'59.5". This avoids having to use the HP41C programs to recompute n if the prism angle is remeasured.
UNCertainty	real		When some, but not all, experimental data points between *BEGIN DATA* and *END DATA* include experimental uncertainties in n, this value is used as the default for points where it is not given. There is no default for this default. If some points include uncertainties, then either all points must, or this default must be nonzero.
ERRor_bar	real		Synonym for *UNCERTAINTY*.

FORMULAS Syntax Between BEGIN and END		
Token #1	Token #2	Description and Defaults
model number	text(72)	Token #1 is an integer. All text following the first token is taken to be token #2, even if it is not enclosed in quotes. Token #2 shows the arithmetic formula used as the model number that is given as token #1. WARNING: MELT is not compiling these formulas. They are just being taken as a text string.

DATA Syntax Between BEGIN and END				
Token #1	Token #2	Token #3	Token #4	Description and Defaults
explicit wavelength	observed index	[index uncertainty]	[expected index]	This option explicitly gives the wavelength λ (in units of microns), and the observed (experimental) index *n*. The experimental uncertainty in index, Δ*n*, is optionally given as token #3, and the nominal index may be given (optionally) as token #4. If token #3 is not given (or zero), and the experimental uncertainty is needed for weighting, then the value given by the *UNCERTAINTY* command is used. If the expected index is given, the manufacturer's dispersion formula will not be used—the stated value will be used instead. All four tokens are reals.
symbolic wavelength	observed index	[index uncertainty]	[expected index]	Same as the previous option, except that the first token is alphabetic. This alphabetic token may be any of the following, representing the standard Fraunhofer wavelengths: i, h, g, F', F, e, d, D, C', C, r, s, t. Note that those involving a single quote must be enclosed by double quotes (e.g., F' is expressed as "F'").
symbolic dispersion	observed dispersion	[index uncertainty of unknown]	[expected index of unknown]	Dispersion is the difference in index from one wavelength to another. Here, the wavelength and index are specified indirectly as a difference from some prior data point. For example, if λ_d and n_d have already been given, "d-C" as token #1 is used to indicate that token #2 is to be interpreted as n_d-n_C, allowing n_C to be determined. In this case, n_C is the "unknown" index. Some vendors report refractometry data in this way so this specification makes data entry from their data sheets simple.
symbolic departure from nominal	observed departure from nominal	[index uncertainty]	[expected index]	Some manufacturers (e.g., Ohara) report refractometry data as a departure from the nominal that is defined by the dispersion formula. To indicate that token #2 is to be interpreted in this way, the symbolic wavelength designation of token #1 is specified as a difference with itself. For example, "d-d" as token #1 means that token #2 is to be interpreted as $n(\lambda_d)$-$n_0(\lambda_d)$. Similarly for "C-C", and so on.

NOMINAL Syntax Between BEGIN and END		
Token #1	Token #2	Description and Defaults
explicit wavelength	expected index	This option explicitly gives the wavelength (in microns) and the index of refraction reported by the manufacturer's catalog as the "expected" value at this wavelength. Values specified in this list will supersede any expected values that are based on the manufacturer's dispersion formula. This is primarily used to specify nominal values for wavelengths outside the domain of the dispersion formula.
symbolic wavelength	expected index	Same as above, except that one of the Fraunhofer designations is used as token #1 instead of a numeric wavelength.

HISTORY Syntax Between BEGIN and END		
Token #1	Token #2	Description and Defaults
model number	occurrences	Both tokens are integers. Token #2 is just a cumulative count of how often the model number (token #1) was used since the history file was begun. Useful for building a histogram.

MELT Commands Controlling Computational Modes & Methods		
Noun	Value	Description and Defaults
WVL	real(7)	Wavelengths, either explicitly given in microns or as symbolic Fraunhofer designations, where the refractive index of the sample is desired. Multiple *WVL* commands may be used to build a list, or up to 7 may be listed on a single line. Explicit numeric values may be mixed with symbolic alphabetic values.
WAVelengths	real(7)	Synonym for *WVL*.
DESign_wvl	real(7)	Synonym for *WVL*.
INDex	real(7)	Expected (nominal) indices for the wavelengths in the *WVL* list. By default, the manufacturer's dispersion formula is used. The *INDEX* list supersedes the results of evaluating the dispersion formula and must be used to specify the expected index for elements of the *WVL* list that are outside the domain of the dispersion formula. The *INDEX* list may be built with multiple commands, or up to 7 indices may be specified on one line. The order of entry must correspond to the order of entry used for the *WVL* specification. If the interpolation model does not rely on a known (expected) index, the *INDEX* specification may be omitted.
MIN_wvl	real	Beginning of the plotting interval. Default is 0.400 μm.
MAX_wvl	real	End of the plotting interval. Default is 0.700 μm.
CONvergence	real	Tolerance on merit function values at the simplex vertices. Default is 0.0001; smaller values make the algorithm work harder to find the minimum.
RISk	real	Controls the width of the computed confidence intervals. Default is 0.05 for 5% risk (95% confidence). Smaller values cause the confidence intervals to be wider.
MFType	integer	1 = Weighted sum of squared residuals (the default); 2 = Weighted sum of absolute deviations; 3 = Weighted maximum deviation; 4 = Chi-square. See page 46 for a discussion of when to use one type instead of another.
MODel	integer(list)	Models are hard-coded and are selected by number. If only a single model number is given, it is simply used. If multiple model numbers are given, all are tried and the "best" is selected according to the criterion described on page 59. The list may be built by specifying an arbitrary number of model numbers on a line (80 characters per line maximum) and/or by specifying an arbitrary number of *MODEL* commands. If model number "0" is encountered in the list, the list is flushed. *MODEL 4* is the default. The list of models may be found in the file MELT.MEL, which is shown in Figure 17 and Figure 18 [page 44 and 45].

• Appendix 8: Matrix Algebra Approach

A matrix algebra approach could be used if the models were always linear in their coefficients, or "transformably" linear. Just such a method is *multiple linear regression.* More than speed* is given up by using the simplex algorithm rather than this more traditional approach: as for all nonlinear methods, the simplex algorithm requires initial starting "guesses" for the unknown coefficients b_k, and the standard error of the coefficients (and other statistics) cannot be computed. The latter has proven to be a serious drawback in assessing the resulting fit and in modifying the model.

Most regression texts present a discussion of the *standard error* of the coefficients, denoted "se(b_k)", but some[93] only cover the topic for the special case of a simple linear model, $y = mx + b$, giving results in a form that yields no clue as to how to extend the concept for more complex models. The general case is presently of interest; it requires a matrix approach to adequately describe it.

First, just why is se(b_k) of interest anyway? Suppose *MODEL 32* is requested of MELT. This model is:

$$n(\lambda) = n_0(\lambda) + \sqrt{b_1 + b_2\lambda^2 + \frac{b_3}{\lambda^2} + \frac{b_4}{\lambda^4} + \frac{b_5}{\lambda^6} + \frac{b_6}{\lambda^8}} \qquad (62)$$

If it is assumed that all these terms are unnecessary, which is very likely, which ones should be omitted? There are 63 unique combinations** of terms; clearly, all cannot

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* Multiple linear regression is not an iterative process, like the simplex algorithm is. The solution is obtained by solving a single matrix equation. The simplex algorithm uses successive approximation to perform a multi-dimensional search for the optimum coefficients; zeroing in on them is like spiraling down a hole with sides of varying steepness (the better the model, the steeper the sides). Hundreds of iterations can be required to find the same solution that the matrix approach can find directly.

** For six terms, taken one at a time, there are 6 different combinations; 15 combinations when taken 2 at a time; 20 when taken 3 at a time; 15 when taken 4 at a time; 6 taken 5 at a time; and 1 taken 6 at a time.

be attempted. By computing a *t-ratio* for each coefficient, those on which the solution does not rely heavily may be identified.

$$t_k = \frac{b_k}{\mathrm{se}(b_k)} \tag{63}$$

When the value of the t-ratio is on the order of unity, or less, then the uncertainty in the value of b_k is as large, or larger, than b_k itself. Intuitively, then, it makes sense to attempt a new solution, this time omitting such coefficients from the model. Generally, the simpler the model the better.

$$\boldsymbol{X}\boldsymbol{b} = \boldsymbol{y}, \text{ where}$$

$$\boldsymbol{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k_{max}} \\ x_{21} & x_{22} & \cdots & x_{2k_{max}} \\ x_{31} & x_{32} & \cdots & x_{3k_{max}} \\ \vdots & \vdots & \vdots & \vdots \\ x_{j_{max}1} & x_{j_{max}2} & \cdots & x_{j_{max}k_{max}} \end{bmatrix}$$

$$\boldsymbol{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{k_{max}} \end{bmatrix} \tag{64}$$

$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{j_{max}} \end{bmatrix}$$

But how are these se(b_k) values computed? The problem needs to be cast into the matrix notation[94] given by Eq. (64). Multiplying both sides of the equation by $\mathbf{X}^T$ yields the *normal equations* for the linear least squares problem,

$$\boldsymbol{X}^T\boldsymbol{y} = (\boldsymbol{X}^T\boldsymbol{X})\boldsymbol{b} \quad . \tag{65}$$

To solve for the coefficient vector **b**, both sides are multiplied by the inverse of the square matrix $\mathbf{X}^T\mathbf{X}$:*

$$\boldsymbol{b} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \quad . \tag{66}$$

The standard error of the kth coefficient, b_k, is a function of the kth diagonal term of the $(\mathbf{X}^T\mathbf{X})^{-1}$ matrix, and the standard deviation of the values of y about x.**

$$\mathrm{se}(b_k) = s_{yx}\sqrt{\left[(\boldsymbol{X}^T\boldsymbol{X})^{-1}\right]_{kk}} \tag{67}$$

Neither of these equations are used in practice due to the numerical instability involved in the matrix inversion; **X** is typically poorly conditioned (nearly singular), so it must be decomposed into factors which are better behaved and, preferably, easily invertible. A more numerically-stable approach will now be described.

Matrix **X**, with dimensions j_{max} x k_{max} (where $j_{max} \geq k_{max}$), may factored and rewritten as the product of three matrices,

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{W}\boldsymbol{V}^T \quad , \tag{68}$$

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* This direct method is not recommended from a numerical stability standpoint. A more stable method, to be discussed later, is equivalent.

** This is denoted s_{yx}. It is a measure of the variation in the calculated values of y that is still unexplained by the regression and may be computed as the square root of the residual mean square:

$$s_{yx} = \sqrt{\mathrm{MS}_{\mathrm{residual}}}$$

where **U** is a j_{max} x k_{max} column-orthogonal matrix;

W is a k_{max} x k_{max} diagonal matrix with positive or zero elements; and

$\mathbf{V}^T$ is the transpose of a k_{max} x k_{max} orthogonal matrix.

The inverse of **X** may be written as the product of the inverses of the factors of **X**, even if **X** is not square,[95]

$$X^{-1} = V \left[\text{diag}\left(\frac{1}{w_k} \right) \right] U^T \quad , \tag{69}$$

since $\mathbf{V}^T$ is orthogonal, its inverse is simply its transpose, **V**;

W is diagonal, so its inverse is a diagonal matrix whose elements are reciprocals of the elements of **W**; and

U is orthogonal, its inverse is simply its transpose, $\mathbf{U}^T$.

This procedure is called *singular value decomposition* (SVD). It is extremely stable, solving problems that cause *Gaussian elimination*, or *LU decomposition* to fail. Embodying many of the recommendations made by reference 76,[96,*] SVD furthermore allows column degeneracies in **X** to be recognized and removed.[**] SVD allows for the identification of linear combinations of variables that do not contribute to the

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* Such as *Householder reduction* to a bidiagonal form, diagonalization by the *QR decomposition* procedure with shifts.

** Press (1986, pp. 54-58, reference 56) describes how the elements of diagonal matrix $\mathbf{W}^{-1}$ should be examined, and adjusted:

The reciprocal of the *condition number* of a matrix is the ratio of the smallest element of $\mathbf{W}^{-1}$ (i.e., smallest $1/w_k$) to the largest. If zero, then the matrix is singular. If nearly zero, then the matrix is *ill-conditioned.* "Nearly" zero means smaller than the floating point precision of the computer (say, 1 x 10^{-6} for Fortran REAL*4, or 1 x 10^{-12} for REAL*8). The largest element of **W** should be found, and then all other elements tested against the product of this element and the floating point precision. If any are found to be smaller than this factor, they should be replaced by zero. And, additionally, when computing $\mathbf{W}^{-1}$ by taking the reciprocals of the elements of **W**, any elements which are zero in **W** are to be zero in $\mathbf{W}^{-1}$, not infinity.

reduction of χ^2. Removing such variables can reduce the standard error of the other coefficients significantly, and only increase χ^2 slightly.

Now the standard error of the kth coefficient may be calculated.[97]

$$\mathrm{se}(b_k) = \sqrt{\sum_{j=1}^{j_{\max}} \left(\frac{V_{kj}}{w_j} \right)^2} \tag{70}$$

It is proper to quote the coefficients as "$b_k \pm \mathrm{se}(b_k)$". They are also used to compute the t-ratio of Eq. (63) so that coefficients which are not crucial to the model may be identified and eliminated in further analyses.

Finally, what exactly is this matrix **X**? If, for example, it is desired to fit *MODEL 32* [Eq. (62)] by this approach, how should the matrix be cast? Writing $\delta n(\lambda)$ for the quantity $n(\lambda)$-$n_0(\lambda)$, and squaring both sides, transforms Eq. (62) into

$$\left[\delta n(\lambda)\right]^2 = b_1 + b_2\lambda^2 + \frac{b_3}{\lambda^2} + \frac{b_4}{\lambda^4} + \frac{b_5}{\lambda^6} + \frac{b_6}{\lambda^8} \quad , \tag{71}$$

which is linear in its coefficients b_1, b_2, ..., b_6. For $j_{\max}$ data points (λ_j, n_j), each having experimental uncertainty Δn_j,* and $k_{\max}$ unknown coefficients,** matrix **X** is written as shown by Eq. (72). Vector **b** in this equation is simply unknown coefficients. Vector **y**, having dimension $j_{\max}$, consists of the transformed experimental data. Equation (64) is rewritten as follows to fit Eq. (62) to experimental data.

* The quantity δn_j also has an uncertainty equal to Δn_j.

** In this example, $k_{\max} = 6$.

$$\begin{bmatrix} \frac{1}{\Delta n_1} & \frac{\lambda_1^2}{\Delta n_1} & \frac{\lambda_1^{-2}}{\Delta n_1} & \frac{\lambda_1^{-4}}{\Delta n_1} & \frac{\lambda_1^{-6}}{\Delta n_1} & \frac{\lambda_1^{-8}}{\Delta n_1} \\ \frac{1}{\Delta n_2} & \frac{\lambda_2^2}{\Delta n_2} & \frac{\lambda_2^{-2}}{\Delta n_2} & \frac{\lambda_2^{-4}}{\Delta n_2} & \frac{\lambda_2^{-6}}{\Delta n_2} & \frac{\lambda_2^{-8}}{\Delta n_2} \\ \frac{1}{\Delta n_3} & \frac{\lambda_3^2}{\Delta n_3} & \frac{\lambda_3^{-2}}{\Delta n_3} & \frac{\lambda_3^{-4}}{\Delta n_3} & \frac{\lambda_3^{-6}}{\Delta n_3} & \frac{\lambda_3^{-8}}{\Delta n_3} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{1}{\Delta n_{j_{max}}} & \frac{\lambda_{j_{max}}^2}{\Delta n_{j_{max}}} & \frac{\lambda_{j_{max}}^{-2}}{\Delta n_{j_{max}}} & \frac{\lambda_{j_{max}}^{-4}}{\Delta n_{j_{max}}} & \frac{\lambda_{j_{max}}^{-6}}{\Delta n_{j_{max}}} & \frac{\lambda_{j_{max}}^{-8}}{\Delta n_{j_{max}}} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix} = \begin{bmatrix} \left(\frac{\delta n_1}{\Delta n_1}\right)^2 \\ \left(\frac{\delta n_2}{\Delta n_2}\right)^2 \\ \left(\frac{\delta n_3}{\Delta n_3}\right)^2 \\ \left(\frac{\delta n_4}{\Delta n_4}\right)^2 \\ \left(\frac{\delta n_5}{\Delta n_5}\right)^2 \\ \left(\frac{\delta n_6}{\Delta n_6}\right)^2 \end{bmatrix} \tag{72}$$

The Δn_j values are replaced by unity if no estimate of the experimental uncertainty is available.

Since all values for the dependent variable, n, are of the same order of magnitude, the weighting errors that would have occurred under this squaring transform may have been negligible. In hindsight, it seems reasonable that the solution for the transformed problem could have been used as a good starting point for final optimization with the nonlinear algorithm. In addition, the ability to compute se(b_k) would greatly simplify the process of evaluating alternate, nested forms of the chosen model.

• Appendix 9: Nested Model Assessment

Nested models are those which are special cases of other, more complex expressions. It is desirable to determine the simplest form—involving the fewest coefficients—that adequately represents the data. Allowing too many coefficients may lead to unwarranted changes in curve shape.

To decide whether the extra degrees of freedom are significant, in going from a "partial" model to a "full" one, the variance explained by these "extra" coefficients is compared to the variance that remains when the full model is used,

$$F = \frac{\mathrm{MS}_{\mathrm{extra}}}{\mathrm{MS}_{\mathrm{full}}} \quad . \tag{73}$$

If this calculated F ratio is less than the critical value,

$$F_{\mathrm{critical}} = F_{\nu_{\mathrm{extra}},\, \nu_{\mathrm{full}},\, \mathrm{risk}} \quad , \tag{74}$$

then the partial model is retained. If greater, then the extra terms are significant and the partial model is rejected in favor of the full model.

This additional partitioning is also done in sum of squares space, just as with a standard ANOVA. For the two models in question, the $\mathrm{SS}_{\mathrm{residual}}$ is computed according to Eq. (45), the smaller-valued one being $\mathrm{SS}_{\mathrm{full}}$ and the larger $\mathrm{SS}_{\mathrm{partial}}$. The extra complexity of the full model explains more of the variation, and is quantified as

$$\mathrm{SS}_{\mathrm{extra}} = \mathrm{SS}_{\mathrm{partial}} - \mathrm{SS}_{\mathrm{full}} \quad . \tag{75}$$

The number of degrees of freedom associated with $\mathrm{SS}_{\mathrm{extra}}$ is denoted $\mathrm{DF}_{\mathrm{extra}}$, computed by subtraction,

$$DF_{extra} = DF_{partial} - DF_{full} \quad , \tag{76}$$

and the mean squares are computed as the ratio of the sum of squares to the degrees of freedom,

$$MS_{full} = \frac{SS_{full}}{DF_{full}} \quad , \text{ and}$$
$$MS_{partial} = \frac{SS_{partial}}{DF_{partial}} \quad . \tag{77}$$

An example using *Sample 2* will now be presented to illustrate nested model analysis. This sample has been previously analyzed, finding *MODEL 32* to be too complex [Figure 21, page 53, and Figure 22, page 56], *MODEL 26* to be too simple [Figure 23, page 56], and *MODEL 21* to be optimum [Figure 26, page 60].

First, consider *MODEL 32* [Eq. (62), page 108] to be the "full" model, and *MODEL 21*,

$$n(\lambda) = n_0(\lambda) + \sqrt{b_1 + \frac{b_2}{\lambda^2}} \quad , \tag{78}$$

to be the "partial" one. The standard ANOVA reports are consulted to obtain the following:

MODEL 32

$SS_{residual}$	$= 4.228 \times 10^{-12}$	$= SS_{full}$
$DF_{residual}$	$= 2$	$= DF_{full}$
$MS_{residual}$	$= 6.140 \times 10^{-13}$	$= MS_{full}$

MODEL 21

$SS_{residual}$	$= 1.020 \times 10^{-11}$	$= SS_{partial}$
$DF_{residual}$	$= 6$	$= DF_{partial}$
$MS_{residual}$	$= 1.700 \times 10^{-12}$	$= MS_{partial}$

EXTRA

SS_{extra}	$= SS_{partial} - SS_{full}$	$= 5.974 \times 10^{-12}$
DF_{extra}	$= DF_{partial} - DF_{full}$	$= 4$
MS_{extra}	$= SS_{extra} \div DF_{extra}$	$= 1.494 \times 10^{-12}$

TEST

$F_{computed}$	$= MS_{extra} \div MS_{full}$	$= 0.707$
$F_{critical}$	$= F_{4,2,.01}$	$= 99.25$

$F_{computed} < F_{critical}$ so the variance accounted for by the extra complexity, in going from the partial model to the full model, is not significant. Keep the partial model.

The nested model analysis agrees with MELT's assessment that *MODEL 21* is preferred to *MODEL 32*.

Now repeat the analysis, this time testing *MODEL 21* as the "full" model and *MODEL 26* [Eq. (25), page 25] as the "partial" expression:

MODEL 21

$SS_{residual}$	$= 1.020 \times 10^{-11}$	$= SS_{full}$
$DF_{residual}$	$= 6$	$= DF_{full}$
$MS_{residual}$	$= 1.700 \times 10^{-12}$	$= MS_{full}$

MODEL 26

$SS_{residual}$	$= 1.218 \times 10^{-10}$	$= SS_{partial}$
$DF_{residual}$	$= 7$	$= DF_{partial}$
$MS_{residual}$	$= 1.740 \times 10^{-11}$	$= MS_{partial}$

EXTRA

SS_{extra}	$= SS_{partial} - SS_{full}$	$= 1.116 \times 10^{-10}$
DF_{extra}	$= DF_{partial} - DF_{full}$	$= 1$
MS_{extra}	$= SS_{extra} \div DF_{extra}$	$= 1.116 \times 10^{-10}$

TEST

$F_{computed}$	$= MS_{extra} \div MS_{full}$	$= 65.62$
$F_{critical}$	$= F_{4,2,.01}$	$= 13.75$

$F_{computed} \geq F_{critical}$ so the variance accounted for by the extra complexity, in going from the partial model to the full model, is significant. The partial model should be rejected in favor of the full model.

This also agrees with the appraisal made by MELT, selecting *MODEL 21* in favor of *MODEL 26*.

• Appendix 10: Weighted Average in Sum of Squares Partitioning

When the w_j weighting factors of Eq. (42) are not the same for all j, then the simple average,

$$\bar{n} = \frac{\sum_{j=1}^{j_{max}} n_j}{j_{max}}, \tag{79}$$

is replaced by the weighted average. This weighted average is computed by adding a correction term to the simple average, as follows:

$$\tilde{n} = \bar{n} + \frac{\sqrt{\sum_{j=1}^{j_{max}} (n_j - \bar{n})^2 - w_j^2 (n_j - \bar{n})^2}}{j_{max}} \tag{80}$$

In a similar way, where Eq. (46) calls for the simple average of the replicated measurements at some λ_j,

$$\bar{n}_j = \frac{\sum_{i=1}^{i_{j,max}} n_{ji}}{i_{j,max}}, \tag{81}$$

the presence of different weights, w_{ji}, makes it necessary to use the weighted average instead:

$$\tilde{n}_j = \bar{n}_j + \frac{\sqrt{\sum_{i=1}^{i_{j,max}} (n_{ji} - \bar{n}_j)^2 - w_{ji}^2 (n_{ji} - \bar{n}_j)^2}}{i_{j,max}} \tag{82}$$

• Appendix 11: Example MELT Analysis with Replicated Data

The replicated data in the following example (*Sample 3*) was acquired by the Author using the Gaertner L123 spectrometer. On page 125 is a plot summarizing the fit of the optimum model to this data.

```
N:\MELTDATA> MELT TEST4.MEL
[<MELT  >-REV5.71]
! MELT.MEL

! Setup file for MELT.EXE

BEGIN FORMULAS

! The following lists the formulas which are coded into the program.  Token #1
! is the model number that is selected with the MODEL keyword.  The remainder
! of the line is token #2.  WARNING: do not change the value of token #1 for a
! model since the program is not compiling the following lines.  Changing the
! formula will have no computational effect; changing the model number will
! indicate that an undesired formula has been used during computation.

!     One-term, one-coefficient models.
26    N  =  N0 + B1

!     Two-term, two-coefficient models.
 1    N  =  N0 + B1 + B2*W
18    N  =  N0 + SQRT( B1 + B2*W )
 2    N  =  N0 + B1 + B2/W
19    N  =  N0 + SQRT( B1 + B2/W )
 3    N  =  N0 + B1 + B2*W^2
20    N  =  N0 + SQRT( B1 + B2*W^2 )
 4    N  =  N0 + B1 + B2/W^2
21    N  =  N0 + SQRT( B1 + B2/W^2 )

!     Two-term, three-coefficient models.
22    N  =  N0 + B1 + B2*W^B3
23    N  =  N0 + SQRT( B1 + B2*W^B3 )
24    N  =  N0 + B1 + B2/W^B3
25    N  =  N0 + SQRT( B1 + B2/W^B3 )

!     Three-term, three-coefficient models.
17    N  =  N0 + B1 + B2*W + B3/W
33    N  =  N0 + SQRT( B1 + B2*W + B3/W )
 5    N  =  N0 + B1 + B2*W + B3*W^2
34    N  =  N0 + SQRT( B1 + B2*W + B3*W^2 )
 6    N  =  N0 + B1 + B2/W + B3/W^2
35    N  =  N0 + SQRT( B1 + B2/W + B3/W^2 )
 7    N  =  N0 + B1 + B2*W^2 + B3*W^4
36    N  =  N0 + SQRT( B1 + B2*W^2 + B3*W^4 )
 8    N  =  N0 + B1 + B2/W^2 + B3/W^4
37    N  =  N0 + SQRT( B1 + B2/W^2 + B3/W^4 )
 9    N  =  N0 + B1 + B2*W^2 + B3/W^2
38    N  =  N0 + SQRT( B1 + B2*W^2 + B3/W^2 )

!     Sellmeier forms; 1- 2- and 3-term, 2- 4- and 6-coefficient.
11    N  =  N0 + SQRT( B2*W^2/(W^2-B1^2) )
12    N  =  N0 + SQRT( B3*W^2/(W^2-B1^2) + B4*W^2/(W^2-B2^2) )
13    N  =  N0 + SQRT( B4*W^2/(W^2-B1^2) + B5*W^2/(W^2-B2^2) + B6*W^2/(W^2-B3^2)

!     Six-term, six coefficient models.
32    N  =  N0 + SQRT( B1 + B2*W^2 + B3/W^2 + B4/W^4 + B5/W^6 + B6/W^8 )

!     Forms not involving a known nominal model, N0.

!     Manufacturers' 6-term, 6-coefficient form.
10    N  =       SQRT( B1 + B2*W^2 + B3/W^2 + B4/W^4 + B5/W^6 + B6/W^8 )

!     Cauchy form.
27    N  =       B1 + B2/W^2 + B3/W^4
```

```
!     Conrady form.
28    N  =        B1 + B2/W + B3/W^3.5

!     Hartman 1, 2, and 3 term.
29    N  =        B1/(W-B2)^B3
30    N  =        B1 + B2/(W-B3)^B4
31    N  =        B1 + B2/(W-B4) + B3/(W-B5)

!     Sellmeier forms; I- 2- and 3-term, 2- 4- and 6-coefficient.
14    N  =  SQRT( 1.0 + B2*W^2/(W^2-B1^2) )
15    N  =  SQRT( 1.0 + B3*W^2/(W^2-B1^2) + B4*W^2/(W^2-B2^2) )
16    N  =  SQRT( 1.0 + B4*W^2/(W^2-B1^2) + B5*W^2/(W^2-B2^2) + B6*W^2/(W^2-B3^2

END FORMULAS

COMPANY 'MELLES GRIOT - ROCHESTER, NY'
MIN_WVL         .4
MAX_WVL         .7
UNCERTAINTY    .0001  ! Assume refractometry from United Lens.
CATALOG          D:\SCIP\GLASDATA\
WVL            .6328  ! Always compute index for HeNe for Zygo.
DEBUG         NO
PLOTTER       ON HP7470A
PLOT          WAVELENGTH
PRINTER       OFF
MODEL       1 18 2 19 3 20 4 21
MODEL       24 25 17 33 5 34 6 35 7 36 8 37 9 38 32
MODEL       11 12 13
MFTYPE       4        ! Chi-Square
CONVERGENCE 1.0E-4   ! smaller values cause simplex optimization to work harder
RISK       .010      ! have MELT quote 99.0% confidence intervals
FFEND      YES       ! In a PC environment, end report with a form-feed.

HISTORY FILE E:\THESIS\MELT\WORK\HISTORY.MEL
HISTORY YES

! TEST4.MEL

PART_NUMBER     31872
LOT    B
PROJECT_NUMBER P-377
GLASS_TYPE      SFL6
MANUFACTURER    SCHOTT
SUPPLIER        UNITED
WAVELENGTHS
MELT    L2115A
ANNEAL  MEG55
FORM    BLOCK
MFTYPE          4
uncertainty     .000010
WVL    D F C
MAX      .750
MIN      .400

BEGIN DATA
! This data was gathered on 4-15-89 by DS on the Gaertner L123.
h       1.865016       !.000050       ! couldn't see the X target -- too dim.
g       1.847478
"F'"    1.830007
"C'"    1.797901
.5085822        1.821652        ! Cd green line
.4678149        1.834203        ! Cd blue line
d       1.805541
.667815         1.795234                ! He red line
r       1.791533
e       1.812983
.576959         1.807257                ! Hg yellow
.579065         1.806911                ! Hg yellow

! This data contrived to plan example of replicated data.
! A random error component was added to each.  This component has a gaussian
! distribution:  mean=0, sdev=0.000010 (HP41C "GN" with pi-3 as the seed).
h           1.865021
g           1.847469
"F'"        1.830030
"C'"        1.797897
```

```
.5085822        1.821655        ! Cd green line
.4678149        1.834197        ! Cd blue line
d           1.805551
.667815         1.795245                ! He red line
r           1.791560
e           1.813003
.576959         1.807253                ! Hg yellow
.579065         1.806908                ! Hg yellow

END DATA

ANGLE   60.21007        60.21282  ! made an error reading the angle

MEL> go

WARNING   The OBSERVED INDEX was altered to compensate for the change
          in prism angle from 60.21007 to 60.21282 degrees (HMS).
```

EXPERIMENTAL WAVELENGTH	DEVIATION ANGLE RADIANS	HMS	OBSERVED INDEX NEW	OLD	CHANGE
.404656(h)	1.377094	78.54060	1.864848	1.865016	-.000168
.404656(h)	1.377108	78.54089	1.864853	1.865021	-.000168
.435834(g)	1.328065	76.05332	1.847315	1.847478	-.000163
.435834(g)	1.328041	76.05281	1.847306	1.847469	-.000163
.467815	1.292870	74.04335	1.834044	1.834203	-.000159
.467815	1.292854	74.04303	1.834038	1.834197	-.000159
.479991(F')	1.282048	73.27214	1.829849	1.830007	-.000158
.479991(F')	1.282107	73.27336	1.829872	1.830030	-.000158
.508582	1.260907	72.14407	1.821499	1.821655	-.000156
.508582	1.260899	72.14392	1.821496	1.821652	-.000156
.546074(e)	1.239481	71.01013	1.812830	1.812983	-.000153
.546074(e)	1.239530	71.01113	1.812850	1.813003	-.000153
.576959	1.225608	70.13199	1.807105	1.807257	-.000152
.576959	1.225599	70.13178	1.807101	1.807253	-.000152
.579065	1.224777	70.10283	1.806759	1.806911	-.000152
.579065	1.224769	70.10268	1.806756	1.806908	-.000152
.587562(d)	1.221491	69.59107	1.805390	1.805541	-.000151
.587562(d)	1.221515	69.59156	1.805400	1.805551	-.000151
.643847(C')	1.203380	68.56549	1.797752	1.797901	-.000149
.643847(C')	1.203370	68.56529	1.797748	1.797897	-.000149
.667815	1.197138	68.35274	1.795085	1.795234	-.000149
.667815	1.197164	68.35328	1.795096	1.795245	-.000149
.706519(r)	1.188544	68.05548	1.791385	1.791533	-.000148
.706519(r)	1.188606	68.06077	1.791412	1.791560	-.000148

MODEL	ITERATIONS	MERIT	F-TEST FOR TERMS OTHER THAN THE MEAN COMPUTED	CRITICAL	RATIO
1	29	5.22E+02	94.573	7.945	11.90
18	69	5.90E+01	1008.652	7.945	126.95
2	29	2.40E+02	231.232	7.945	29.10
19	64	4.63E+01	1291.581	7.945	162.56
3	32	6.89E+02	66.198	7.945	8.33
20	61	9.29E+01	632.120	7.945	79.56
4	32	1.40E+02	411.967	7.945	51.85
21	68	6.16E+01	964.284	7.945	121.36
24	197	2.54E+01	1133.424	5.780	196.08
25	656	4.96E+01	574.503	5.780	99.39
17	105	4.71E+01	605.964	5.780	104.83
33	86	4.33E+01	659.558	5.780	114.10
5	81	8.49E+01	331.442	5.780	57.34
34	83	5.90E+01	481.401	5.780	83.28
6	80	3.19E+01	898.141	5.780	155.38
35	109	4.36E+01	654.785	5.780	113.28
7	86	1.44E+02	191.077	5.780	33.06
36	90	4.38E+01	651.144	5.780	112.65
8	52	2.61E+01	1098.874	5.780	190.10
37	123	4.63E+01	616.834	5.780	106.71
9	68	4.17E+01	685.967	5.780	118.67
38	95	5.53E+01	514.293	5.780	88.97
32	237	3.65E+01	268.994	4.248	63.32
11	46	2.76E+03	-.001	7.945	.00
12	84	7.96E+01	224.880	4.938	45.54

13	241	4.34E+01	225.499	4.248	53.09

MODEL 24, using 3 out of 24 degrees-of-freedom, is optimum.

R E F R A C T O M E T R Y A N A L Y S I S

PART NUMBER:	31872	MATERIAL FORM:	BLOCK	MODEL NUM:	24
PROJECT NUMBER:	P-377	SUPPLIER:	UNITED	MFTYPE NUM:	4
MANUFACTURER:	SCHOTT	MELT NUMBER:	L2115A	ITERATIONS:	197
GLASS TYPE:	SFL6	ANNEAL NUMBER:	MEG55	MERIT:	2.5E+01
LOT NAME:	B	ANALYSIS DATE:	02-17-90	CONVERGENCE:	1.0E-04

DESIGN WAVELENGTH	INTERPOLATED INDEX	NOMINAL INDEX	ERROR FROM NOMINAL	+/- 99.0% CONFIDENCE INTERVALS
.486133(F)	1.827909	1.827798	.000111	.000066
.589294(D)	1.805118	1.804909	.000209	.000066
.632800	1.799062	1.798835	.000228	.000067
.656272(C)	1.796325	1.796090	.000235	.000067

EXPERIMENTAL WAVELENGTH	OBSERVED INDEX	INTERPOLATED INDEX	RESIDUAL	+/- 99.0% CONFIDENCE INTERVALS
.404656(h)	1.864848	1.864852	-.000004	.000069
.404656(h)	1.864853	1.864852	.000001	.000069
.435834(g)	1.847315	1.847312	.000004	.000068
.435834(g)	1.847306	1.847312	-.000005	.000068
.467815	1.834044	1.834033	.000011	.000067
.467815	1.834038	1.834033	.000005	.000067
.479991(F')	1.829849	1.829863	-.000014	.000066
.479991(F')	1.829872	1.829863	.000009	.000066
.508582	1.821499	1.821499	.000000	.000066
.508582	1.821496	1.821499	-.000003	.000066
.546074(e)	1.812830	1.812833	-.000004	.000066
.546074(e)	1.812850	1.812833	.000016	.000066
.576959	1.807105	1.807120	-.000014	.000066
.576959	1.807101	1.807120	-.000018	.000066
.579065	1.806759	1.806768	-.000008	.000066
.579065	1.806756	1.806768	-.000011	.000066
.587562(d)	1.805390	1.805391	-.000001	.000066
.587562(d)	1.805400	1.805391	.000009	.000066
.643847(C')	1.797752	1.797734	.000018	.000067
.643847(C')	1.797748	1.797734	.000014	.000067
.667815	1.795085	1.795090	-.000005	.000068
.667815	1.795096	1.795090	.000006	.000068
.706519(r)	1.791385	1.791402	-.000017	.000069
.706519(r)	1.791412	1.791402	.000010	.000069

EXPERIMENTAL WAVELENGTH	OBSERVED INDEX	NOMINAL INDEX	ERROR FROM NOMINAL	STATED EXPERIMENTAL UNCERTAINTY	MERIT FUNCTION WEIGHT
.404656(h)	1.864848	1.864973	-.000125	.000010	1.000000
.404656(h)	1.864853	1.864973	-.000120	.000010	1.000000
.435834(g)	1.847315	1.847314	.000002	.000010	1.000000
.435834(g)	1.847306	1.847314	-.000007	.000010	1.000000
.467815	1.834044	1.833955	.000089	.000010	1.000000
.467815	1.834038	1.833955	.000083	.000010	1.000000
.479991(F')	1.829849	1.829762	.000087	.000010	1.000000
.479991(F')	1.829872	1.829762	.000110	.000010	1.000000
.508582	1.821499	1.821356	.000143	.000010	1.000000
.508582	1.821496	1.821356	.000140	.000010	1.000000
.546074(e)	1.812830	1.812653	.000177	.000010	1.000000
.546074(e)	1.812850	1.812653	.000197	.000010	1.000000
.576959	1.807105	1.806918	.000188	.000010	1.000000
.576959	1.807101	1.806918	.000184	.000010	1.000000
.579065	1.806759	1.806564	.000195	.000010	1.000000
.579065	1.806756	1.806564	.000192	.000010	1.000000
.587562(d)	1.805390	1.805182	.000207	.000010	1.000000

.587562(d)	1.805400	1.805182	.000217	.000010	1.000000
.643847(C')	1.797752	1.797503	.000249	.000010	1.000000
.643847(C')	1.797748	1.797503	.000245	.000010	1.000000
.667815	1.795085	1.794852	.000233	.000010	1.000000
.667815	1.795096	1.794852	.000244	.000010	1.000000
.706519(r)	1.791385	1.791156	.000229	.000010	1.000000
.706519(r)	1.791412	1.791156	.000256	.000010	1.000000

WARNING - The OBSERVED INDEX was altered to compensate for the change in prism angle from 60.21007 to 60.21282 degrees (HMS).

EXPERIMENTAL WAVELENGTH	DEVIATION ANGLE RADIANS	HMS	OBSERVED INDEX NEW	OLD	CHANGE
.404656(h)	1.377094	78.54060	1.864848	1.865016	-.000168
.404656(h)	1.377108	78.54089	1.864853	1.865021	-.000168
.435834(g)	1.328065	76.05332	1.847315	1.847478	-.000163
.435834(g)	1.328041	76.05281	1.847306	1.847469	-.000163
.467815	1.292870	74.04335	1.834044	1.834203	-.000159
.467815	1.292854	74.04303	1.834038	1.834197	-.000159
.479991(F')	1.282048	73.27214	1.829849	1.830007	-.000158
.479991(F')	1.282107	73.27336	1.829872	1.830030	-.000158
.508582	1.260907	72.14407	1.821499	1.821655	-.000156
.508582	1.260899	72.14392	1.821496	1.821652	-.000156
.546074(e)	1.239481	71.01013	1.812830	1.812983	-.000153
.546074(e)	1.239530	71.01113	1.812850	1.813003	-.000153
.576959	1.225608	70.13199	1.807105	1.807257	-.000152
.576959	1.225599	70.13178	1.807101	1.807253	-.000152
.579065	1.224777	70.10283	1.806759	1.806911	-.000152
.579065	1.224769	70.10268	1.806756	1.806908	-.000152
.587562(d)	1.221491	69.59107	1.805390	1.805541	-.000151
.587562(d)	1.221515	69.59156	1.805400	1.805551	-.000151
.643847(C')	1.203380	68.56549	1.797752	1.797901	-.000149
.643847(C')	1.203370	68.56529	1.797748	1.797897	-.000149
.667815	1.197138	68.35274	1.795085	1.795234	-.000149
.667815	1.197164	68.35328	1.795096	1.795245	-.000149
.706519(r)	1.188544	68.05548	1.791385	1.791533	-.000148
.706519(r)	1.188606	68.06077	1.791412	1.791560	-.000148

A N A L Y S I S O F V A R I A N C E

SOURCES	RELATIVE SS	DF	MS=SS/DF
TOTAL (UNCORRECTED)	1.000000	24	
REGRESSION (DUE TO THE MEAN)	.637562	1	4.86092E-07
TOTAL (CORRECTED FOR THE MEAN)	.362438	23	1.20144E-08
REGRESSION (EXCLUDING THE MEAN)	.359112	2	1.36898E-07
RESIDUAL	.003327	21	1.20782E-10
ERROR	.001360	12	8.64340E-11
LACK-OF-FIT	.001966	9	1.66578E-10

CORRELATION COEFFICIENT

DUE TO THE MEAN = .6376

This implies that approximately 63.76% of the total variation in the data is explained by a regression term representing the mean.

EXCLUDING THE MEAN = .9908

This implies that approximately 99.08% of the remaining variation in the data is explained by regression terms other than the mean.

```
F-TESTS FOR SIGNIFICANCE OF THE REGRESSION
==========================================

  DUE TO THE MEAN
  ---------------
     F(observed)  =  REGRESSION_MS /  TOTAL_MS     =   40.46

     F(critical)  =  F(  1, 23, .010)              =   7.881

     F(observed)  >  F(critical) implies that a significant amount of
     variation in the data is explained by a regression term
     representing the mean.  This term should not be rejected.

  EXCLUDING THE MEAN
  ------------------
     F(observed)  =  REGRESSION_MS / RESIDUAL_MS  =   1133.

     F(critical)  =  F(  2, 21, .010)             =   5.780

     F(observed)  >  F(critical) implies that a significant amount of
     the remaining variation in the data is explained by regression
     terms other than the mean.  These terms should not be rejected.


F-TEST FOR SIGNIFICANT LACK-OF-FIT
==================================

     F(observed)  =  LOF_MS / ERROR_MS  =   1.927

     F(critical)  =  F(  9, 12, .010)   =   4.388

     F(observed)  <  F(critical) implies that the lack-of-fit of the
     model to the data is insignificant compared to the errors in the
     measurements.  The model does not need to be rejected.

MFTYPE  Description                              VALUE
======  ================================      ==========

     1  WEIGHTED SUM-OF-SQUARED RESIDUALS
     2  WEIGHTED SUM-OF-ABSOLUTE RESIDUALS
     3  WEIGHTED MAXIMUM DEVIATION
 --> 4  CHI-SQUARE                              25.36


CHI-SQUARE ANALYSIS
===================

Guidelines for CHI-SQUARE:
--------------------------
    The better the fit, the lower the CHI-SQUARE.  The more statistically
    significant the fit, the closer the probability Q will be to 1.0

    For a "moderately" good fit, CHI-SQUARE should be approximately equal to
    the number of degrees-of-freedom.  Here, the ratio of degrees-of-freedom
    to CHI-SQUARE is  .828    ; the goal is unity.


Guidelines for Q:
-----------------
    The probability, Q, that CHI-SQUARE for the correct model could be even
    larger if the residual variation is really due only to chance is  .232

    Q >  0.9       Possibly non-experimental data (fit is too good to be
                   the result of experiment), or grossly over estimated
                   uncertainties (too conservative).

    Q >  0.1       Reasonable for real-world data when the model is correct,
                   especially if the uncertainties are not normally
                   distributed (an abundance of outlier points may have
                   resulted).  If always on this order of magnitude, then
                   the uncertainties may be slightly under estimated, the
                   model may be marginal, or the uncertainties may be
                   inherently skewed or otherwise non-normal.

    Q << 0.001     Indicates that the model is wrong, or the uncertainties
```

```
                    are grossly under estimated.


MODEL Formula
===== ========================================================================

   26 N  =  N0 + B1
    1 N  =  N0 + B1 + B2*W
   18 N  =  N0 + SQRT( B1 + B2*W )
    2 N  =  N0 + B1 + B2/W
   19 N  =  N0 + SQRT( B1 + B2/W )
    3 N  =  N0 + B1 + B2*W^2
   20 N  =  N0 + SQRT( B1 + B2*W^2 )
    4 N  =  N0 + B1 + B2/W^2
   21 N  =  N0 + SQRT( B1 + B2/W^2 )
   22 N  =  N0 + B1 + B2*W^B3
   23 N  =  N0 + SQRT( B1 + B2*W^B3 )
-->24 N  =  N0 + B1 + B2/W^B3
   25 N  =  N0 + SQRT( B1 + B2/W^B3 )
   17 N  =  N0 + B1 + B2*W + B3/W
   33 N  =  N0 + SQRT( B1 + B2*W + B3/W )
    5 N  =  N0 + B1 + B2*W + B3*W^2
   34 N  =  N0 + SQRT( B1 + B2*W + B3*W^2 )
    6 N  =  N0 + B1 + B2/W + B3/W^2
   35 N  =  N0 + SQRT( B1 + B2/W + B3/W^2 )
    7 N  =  N0 + B1 + B2*W^2 + B3*W^4
   36 N  =  N0 + SQRT( B1 + B2*W^2 + B3*W^4 )
    8 N  =  N0 + B1 + B2/W^2 + B3/W^4
   37 N  =  N0 + SQRT( B1 + B2/W^2 + B3/W^4 )
    9 N  =  N0 + B1 + B2*W^2 + B3/W^2
   38 N  =  N0 + SQRT( B1 + B2*W^2 + B3/W^2 )
   11 N  =  N0 + SQRT( B2*W^2/(W^2-B1^2) )
   12 N  =  N0 + SQRT( B3*W^2/(W^2-B1^2) + B4*W^2/(W^2-B2^2) )
   13 N  =  N0 + SQRT( B4*W^2/(W^2-B1^2) + B5*W^2/(W^2-B2^2) + B6*W^2/(W^2-B3^2)
   32 N  =  N0 + SQRT( B1 + B2*W^2 + B3/W^2 + B4/W^4 + B5/W^6 + B6/W^8 )
   10 N  =       SQRT( B1 + B2*W^2 + B3/W^2 + B4/W^4 + B5/W^6 + B6/W^8 )
   27 N  =       B1 + B2/W^2 + B3/W^4
   28 N  =       B1 + B2/W + B3/W^3.5
   29 N  =       B1/(W-B2)^B3
   30 N  =       B1 + B2/(W-B3)^B4
   31 N  =       B1 + B2/(W-B4) + B3/(W-B5)
   14 N  =  SQRT( 1.0 + B2*W^2/(W^2-B1^2) )
   15 N  =  SQRT( 1.0 + B3*W^2/(W^2-B1^2) + B4*W^2/(W^2-B2^2) )
   16 N  =  SQRT( 1.0 + B4*W^2/(W^2-B1^2) + B5*W^2/(W^2-B2^2) + B6*W^2/(W^2-B3^2)


Model Coefficients
======================

   B1  =   2.725444E-04
   B2  =  -4.880877E-06
   B3  =   4.851608E+00


[<MELT  >-REV5.71]

Updating history file MELTHIST.TXT. . .

Sending plotter instructions to TEST4.PLT for HP7470A . . .

Updating history file E:\THESIS\MELT\WORK\HISTORY.MEL. . .


N:\MELTDATA>
```

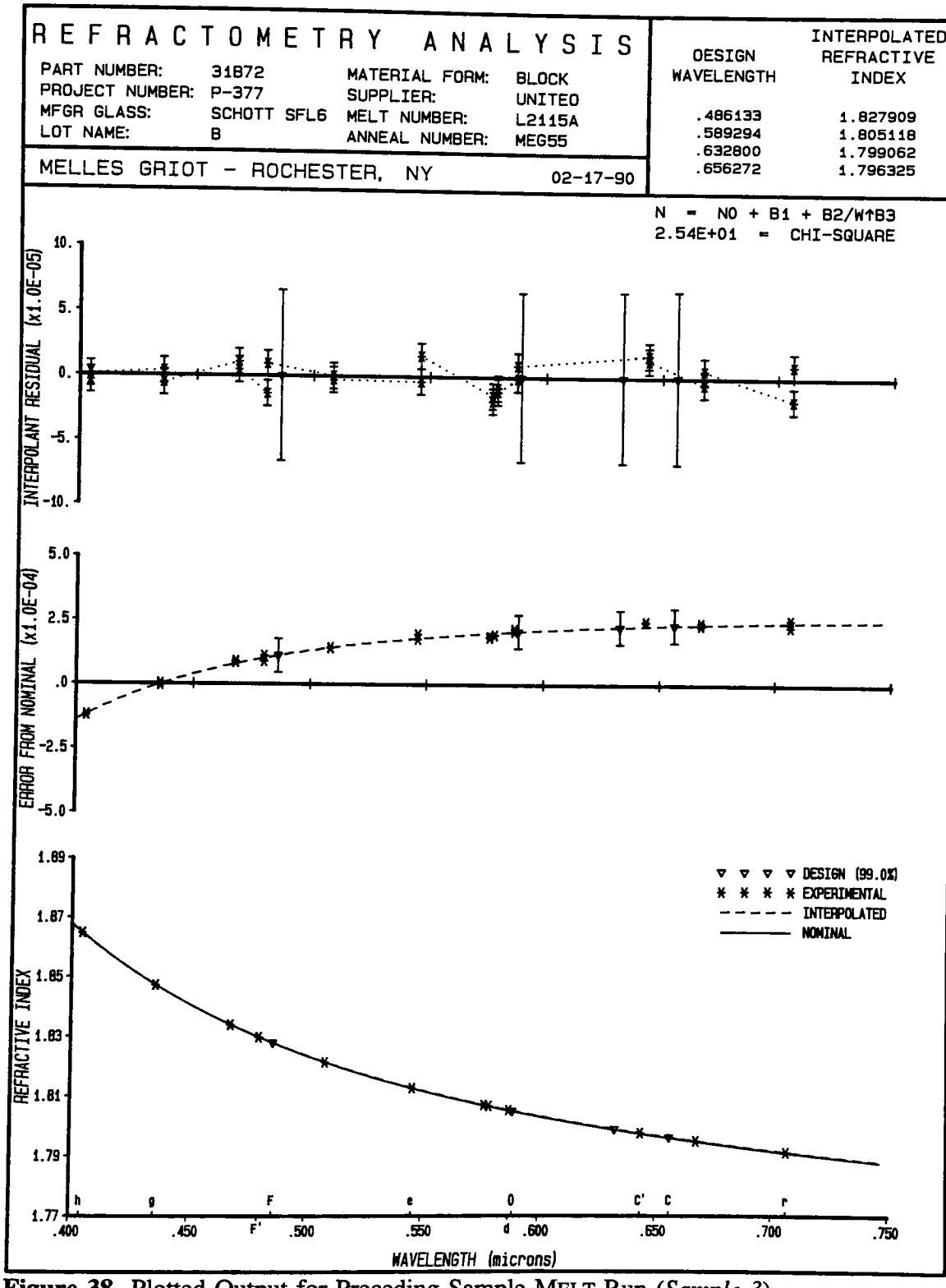

Figure 38 Plotted Output for Preceding Sample MELT Run (*Sample 3*)

• Appendix 12: MELT Output for Figure 28 & Figure 29

The MELT output which follows corresponds to the plotted output presented in Figure 28 [page 68] in the Discussion section for *Sample 4*.

R E F R A C T O M E T R Y A N A L Y S I S

PART NUMBER:	OG-3710	MATERIAL FORM:	PRESSINGS	MODEL NUM:	4
PROJECT NUMBER:	unspecified	SUPPLIER:	OHARA-USA	MFTYPE NUM:	4
MANUFACTURER:	OHARA	MELT NUMBER:	J506822	ITERATIONS:	40
GLASS TYPE:	SFL6	ANNEAL NUMBER:	313	MERIT:	1.8E-01
LOT NAME:	unspecified	ANALYSIS DATE:	02-19-90	CONVERGENCE:	1.0E-04

DESIGN WAVELENGTH	INTERPOLATED INDEX	NOMINAL INDEX	ERROR FROM NOMINAL	+/- 95.0% CONFIDENCE INTERVALS
.450000	1.840963	1.840864	.000099	.000016
.550000	1.811991	1.811849	.000142	.000014
.632800	1.799006	1.798843	.000164	.000016
.650000	1.796970	1.796803	.000167	.000017

EXPERIMENTAL WAVELENGTH	OBSERVED INDEX	INTERPOLATED INDEX	RESIDUAL	+/- 95.0% CONFIDENCE INTERVALS
.435834(g)	1.847333	1.847334	-.000001	.000016
.486133(F)	1.827882	1.827880	.000002	.000015
.587562(d)	1.805331	1.805334	-.000003	.000015
.656272(C)	1.796272	1.796270	.000002	.000017

EXPERIMENTAL WAVELENGTH	OBSERVED INDEX	NOMINAL INDEX	ERROR FROM NOMINAL	STATED EXPERIMENTAL UNCERTAINTY	MERIT FUNCTION WEIGHT
.435834(g)	1.847333	1.847243	.000090	.000010	1.000000
.486133(F)	1.827882	1.827762	.000120	.000010	1.000000
.587562(d)	1.805331	1.805181	.000150	.000010	1.000000
.656272(C)	1.796272	1.796102	.000170	.000010	1.000000

A N A L Y S I S O F V A R I A N C E

SOURCES	RELATIVE SS	DF	MS=SS/DF
TOTAL (UNCORRECTED)	1.000000	4	
REGRESSION (DUE TO THE MEAN)	.950312	1	7.02262E-08
TOTAL (CORRECTED FOR THE MEAN)	.049688	3	1.22396E-09
REGRESSION (EXCLUDING THE MEAN)	.049447	1	3.65402E-09
RESIDUAL	.000242	2	8.92460E-12

CORRELATION COEFFICIENT

DUE TO THE MEAN = .9503

This implies that approximately 95.03% of the total variation in the data is explained by a regression term representing the mean.

EXCLUDING THE MEAN = .9951

This implies that approximately 99.51% of the remaining variation in the data is explained by regression terms other than the mean.

F-TESTS FOR SIGNIFICANCE OF THE REGRESSION

DUE TO THE MEAN

F(observed) = REGRESSION_MS / TOTAL_MS = 57.38

F(critical) = F(1, 3, .050) = 10.13

F(observed) > F(critical) implies that a significant amount of variation in the data is explained by a regression term representing the mean. This term should not be rejected.

EXCLUDING THE MEAN

F(observed) = REGRESSION_MS / RESIDUAL_MS = 409.4

F(critical) = F(1, 2, .050) = 18.51

F(observed) > F(critical) implies that a significant amount of the remaining variation in the data is explained by regression terms other than the mean. These terms should not be rejected.

MFTYPE	Description	VALUE
1	WEIGHTED SUM-OF-SQUARED RESIDUALS	
2	WEIGHTED SUM-OF-ABSOLUTE RESIDUALS	
3	WEIGHTED MAXIMUM DEVIATION	
--> 4	CHI-SQUARE	.1785

CHI-SQUARE ANALYSIS

Guidelines for CHI-SQUARE:

The better the fit, the lower the CHI-SQUARE. The more statistically significant the fit, the closer the probability Q will be to 1.0

For a "moderately" good fit, CHI-SQUARE should be approximately equal to the number of degrees-of-freedom. Here, the ratio of degrees-of-freedom to CHI-SQUARE is 11.2 ; the goal is unity.

Guidelines for Q:

The probability, Q, that CHI-SQUARE for the correct model could be even larger if the residual variation is really due only to chance is .915

Q > 0.9	Possibly non-experimental data (fit is too good to be the result of experiment), or grossly over estimated uncertainties (too conservative).
Q > 0.1	Reasonable for real-world data when the model is correct, especially if the uncertainties are not normally distributed (an abundance of outlier points may have resulted). If always on this order of magnitude, then the uncertainties may be slightly under estimated, the model may be marginal, or the uncertainties may be inherently skewed or otherwise non-normal.
Q << 0.001	Indicates that the model is wrong, or the uncertainties are grossly under estimated.

The MELT output which follows corresponds to the plotted output presented in Figure 29 [page 68] in the Discussion section for *Sample 5*.

R E F R A C T O M E T R Y A N A L Y S I S

PART NUMBER:	OG-3710	MATERIAL FORM:	PRESSINGS	MODEL NUM:	4
PROJECT NUMBER:	unspecified	SUPPLIER:	OHARA-USA	MFTYPE NUM:	4
MANUFACTURER:	OHARA	MELT NUMBER:	J506822	ITERATIONS:	34
GLASS TYPE:	SFL6	ANNEAL NUMBER:	314	MERIT:	2.4E+00
LOT NAME:	unspecified	ANALYSIS DATE:	02-19-90	CONVERGENCE:	1.0E-04

DESIGN WAVELENGTH	INTERPOLATED INDEX	NOMINAL INDEX	ERROR FROM NOMINAL	+/- 95.0% CONFIDENCE INTERVALS
.450000	1.840640	1.840864	-.000224	.000058
.550000	1.811721	1.811849	-.000128	.000053
.632800	1.798762	1.798843	-.000081	.000058
.650000	1.796730	1.796803	-.000073	.000060

EXPERIMENTAL WAVELENGTH	OBSERVED INDEX	INTERPOLATED INDEX	RESIDUAL	+/- 95.0% CONFIDENCE INTERVALS
.435834(g)	1.846993	1.847000	-.000007	.000060
.486133(F)	1.827592	1.827579	.000013	.000055
.587562(d)	1.805071	1.805076	-.000006	.000054
.656272(C)	1.796032	1.796031	.000000	.000061

EXPERIMENTAL WAVELENGTH	OBSERVED INDEX	NOMINAL INDEX	ERROR FROM NOMINAL	STATED EXPERIMENTAL UNCERTAINTY	MERIT FUNCTION WEIGHT
.435834(g)	1.846993	1.847243	-.000250	.000010	1.000000
.486133(F)	1.827592	1.827762	-.000170	.000010	1.000000
.587562(d)	1.805071	1.805181	-.000110	.000010	1.000000
.656272(C)	1.796032	1.796102	-.000070	.000010	1.000000

A N A L Y S I S O F V A R I A N C E

SOURCES	RELATIVE SS	DF	MS=SS/DF
TOTAL (UNCORRECTED)	1.000000	4	
REGRESSION (DUE TO THE MEAN)	.830268	1	8.99941E-08
TOTAL (CORRECTED FOR THE MEAN)	.169732	3	6.13251E-09
REGRESSION (EXCLUDING THE MEAN)	.167536	1	1.81595E-08
RESIDUAL	.002196	2	1.19035E-10

CORRELATION COEFFICIENT

DUE TO THE MEAN = .8303

This implies that approximately 83.03% of the total variation in the data is explained by a regression term representing the mean.

EXCLUDING THE MEAN = .9871

This implies that approximately 98.71% of the remaining variation in the data is explained by regression terms other than the mean.

```
F-TESTS FOR SIGNIFICANCE OF THE REGRESSION
==========================================

  DUE TO THE MEAN
  ---------------
     F(observed)  =  REGRESSION_MS /  TOTAL_MS     =   14.67

     F(critical)  =  F(  1,  3, .050)              =   10.13

     F(observed)  >  F(critical) implies that a significant amount of
     variation in the data is explained by a regression term
     representing the mean.  This term should not be rejected.

  EXCLUDING THE MEAN
  ------------------
     F(observed)  =  REGRESSION_MS / RESIDUAL_MS  =   152.6

     F(critical)  =  F(  1,  2, .050)             =   18.51

     F(observed)  >  F(critical) implies that a significant amount of
     the remaining variation in the data is explained by regression
     terms other than the mean.  These terms should not be rejected.

MFTYPE  Description                              VALUE
======  ================================     ==========

     1  WEIGHTED SUM-OF-SQUARED RESIDUALS
     2  WEIGHTED SUM-OF-ABSOLUTE RESIDUALS
     3  WEIGHTED MAXIMUM DEVIATION
 --> 4  CHI-SQUARE                             2.381


CHI-SQUARE ANALYSIS
===================

Guidelines for CHI-SQUARE:
--------------------------
    The better the fit, the lower the CHI-SQUARE.  The more statistically
    significant the fit, the closer the probability Q will be to 1.0

    For a "moderately" good fit, CHI-SQUARE should be approximately equal to
    the number of degrees-of-freedom.  Here, the ratio of degrees-of-freedom
    to CHI-SQUARE is  .840    ; the goal is unity.


Guidelines for Q:
-----------------
    The probability, Q, that CHI-SQUARE for the correct model could be even
    larger if the residual variation is really due only to chance is  .304

    Q >  0.9        Possibly non-experimental data (fit is too good to be
                    the result of experiment), or grossly over estimated
                    uncertainties (too conservative).

    Q >  0.1        Reasonable for real-world data when the model is correct,
                    especially if the uncertainties are not normally
                    distributed (an abundance of outlier points may have
                    resulted).  If always on this order of magnitude, then
                    the uncertainties may be slightly under estimated, the
                    model may be marginal, or the uncertainties may be
                    inherently skewed or otherwise non-normal.

    Q << 0.001      Indicates that the model is wrong, or the uncertainties
                    are grossly under estimated.
```

• Appendix 13: MELT Program Listing

Those modules listed below, with an "*" following their names, are listed in this Appendix (though uncommented to save space). Those with "pltlib" are from a custom plot library (written by the Author); "lib" indicates elements of the Author's custom math and statistics libraries; "nrlib" modules are elements distributed with *Numerical Recipes.*[98] The balance of the routines, with no designation following their names, are special routines written specifically for MELT and are not part of any general library. Listing all modules would double or triple the size of this disertation. Contact the Author if further information is desired.

ABSDIR	pltlib	IP1IP2	pltlib	SILICA	
ABSOLE	pltlib	IVTOR	pltlib	SIZE	pltlib
ADDTON		LENSTR	lib	SORT2D	lib
ADN		LINTYP	pltlib	SORT2DR4	lib
AMOEBA	nrlib	LTJUST	lib	SPACES	pltlib
AMOEBA0	lib	MELT	*	SPAWN	lib
ANOVA	lib	MERITF		SPEED	pltlib
BETACF	nrlib	NEWSUF	lib	STRAIT	pltlib
BETAI	nrlib	NOCRLF	lib	SUBIND	lib
BOLD	pltlib	NOMDAT		SYMOFF	pltlib
CINTER	lib	NOMIND		SYMON	pltlib
CMDARG	lib	P1P2	pltlib	SYSDAT	lib
DEG	lib	PARSEC	lib	SYSDEL	lib
DIASIZ	pltlib	PARSER	lib	TEXT	pltlib
DMODEL		PARSFILE	lib	TPOSE4	lib
DNEWTN	lib	PENDN	pltlib	TRIANG	pltlib
ENDPLT	pltlib	PENUP	pltlib	TTABLE	lib
ERRBAR	pltlib	PLOT1		UM2HZ	lib
FITIND		PLOT2		UPCASE	lib
FTABLE	lib	PLOTDN	pltlib	USERDATA	*
GAMMLN	nrlib	PLOTUP	pltlib	VSQRT	lib
GAMMQ	nrlib	POST	*	WINDOW	pltlib
GCF	nrlib	PREFIT	*	XAXIS	pltlib
GETSYM		RAD	lib	XTIC	pltlib
GSER	nrlib	RELATV	pltlib	XYSCAL	pltlib
HMS2HR	lib	REPORT		YAXIS	pltlib
HR2HMS	lib	REVPRT	lib		
HZ2UM	lib	SCHOTT			
INIT	pltlib	SELECT	pltlib		

```
      PROGRAM MELT
      CHARACTER*6  PROGNAME
      CHARACTER*6  CERR
      CHARACTER*4  REVLEV
      CHARACTER*1  KBELL
      PARAMETER    (PROGNAME = 'MELT  ', REVLEV = '5.71')
      REAL*4       MERITF, AMOEBA0
      REAL*4       TEMP1, TEMP2, TEMP3, TEMP4, FCOMP, FCRIT
      REAL*4       FRATIO, BEST_FRATIO
      INTEGER*4    BEST_MODEL, LOOP
      INTEGER*4    CONSTANT
      PARAMETER    (CONSTANT=26)
      EXTERNAL     MERITF
      INTEGER*2    I, J
      INTEGER*2    LENSTR
$INCLUDE: 'SYMBOLB.FTN'
$INCLUDE: 'SYMBOLC.FTN'
$INCLUDE: 'SYMBOLG.FTN'
$INCLUDE: 'COMMONA.FTN'
$INCLUDE: 'COMMONB.FTN'
$INCLUDE: 'COMMONF.FTN'
$INCLUDE: 'COMMONG.FTN'
      REAL*4       VERTEX, MFVCT
      REAL*4       WORK
      DIMENSION    VERTEX(IBMAX,IBMAX+1), MFVCT(IBMAX+1)
      DIMENSION    WORK(IBMAX*(IBMAX+1))
      KBELL        = CHAR(7)
      DEBUG        = .FALSE.
      IERR         = NO_ERROR
      OPTNAM       = PROGNAME
      OPTREV       = REVLEV
      CALL REVPRT (INT2(KOUT),PROGNAME,REVLEV)
      CALL SYSDAT (I8DATE,INT2(8))
      OPEN (IFILE3,STATUS='NEW',FORM='UNFORMATTED')
      CALL PREFIT (VERTEX)
      IF (IERR .EQ. NO_ERROR) THEN
          IF (MODLIST .EQ. 0) THEN
              WRITE (IFILE3) MODEL
              MODLIST = 1
          ENDIF
          REWIND IFILE3
          IF (MODLIST .GT. 1) WRITE (KOUT,197)
 197      FORMAT(2(/),T43,'F-TEST FOR TERMS OTHER THAN THE MEAN',/,
     +           1X,'MODEL',2X,'ITERATIONS',T30,'MERIT',T43,
     +           'COMPUTED',T57,'CRITICAL',T74,'RATIO',/,1X)
          DO 259  LOOP=1, MODLIST
              READ (IFILE3) MODEL
              CALL DMODEL (VERTEX, B)
              IDF      = IPTS   NUM_B
              IF (IDF .GT. 0) THEN
                  DO 239 J=2, NUM_B+1
                      DO 229 I=1, NUM_B
                          VERTEX(I,J) = 0.0
 229                      CONTINUE
 239                  CONTINUE
                  MERIT    = AMOEBA0(VERTEX,MFVCT,IBMAX,NUM_B,IBMAX+1,
     +                               CONVERGENCE,MERITF,NUMITR,B,WORK)
                  IF (ICOM .EQ. COMPUTE_INDEX_ERROR) THEN
                      CALL ANOVA (-1, NUM_B, IPTS, WVL, ERRN, TERMS,
     +                            WEIGHT, RISK, FCOMP, FCRIT,
     +                            TEMP1, TEMP2, TEMP3, TEMP4)
                  ELSEIF (ICOM .EQ. COMPUTE_INDEX) THEN
                      CALL ANOVA (-1, NUM_B, IPTS, WVL, OBSN, TERMS,
     +                            WEIGHT, RISK, FCOMP, FCRIT,
     +                            TEMP1, TEMP2, TEMP3, TEMP4)
                  ENDIF
                  IF (FCRIT .NE. 0.0) THEN
                      FRATIO  = FCOMP/FCRIT
                  ELSE
                      FRATIO  = 0.0
                  ENDIF
                  IF (MODLIST .GT. 1) THEN
                      WRITE (KOUT,241) MODEL, NUMITR, MERIT, FCOMP,
     +                                 FCRIT, FRATIO
```

```
241                 FORMAT(2X,I4,6X,I6,7X,1PE9.2,2X,2(5X,0PF9.3),5X,
   +                        F9.2)
                ENDIF
                IF (LOOP .GT. 1) THEN
                    IF (FRATIO .GT. BEST_FRATIO) THEN
                        BEST_MODEL  = MODEL
                        BEST_FRATIO = FRATIO
                    ENDIF
                ELSE
                    BEST_MODEL  = MODEL
                    BEST_FRATIO = FRATIO
                ENDIF
            ELSE
                IF (MODLIST .GT. 1) THEN
                    WRITE (KOUT,223) MODEL
223                 FORMAT(1X,'WARNING - Skipping MODEL',I4,' due ',
   +                        'to insufficient degrees-of-freedom.')
                ELSE
                    IERR    = NO_DEGREES_OF_FREEDOM
                ENDIF
            ENDIF
259         CONTINUE
        IF (IERR .EQ. NO_ERROR) THEN
            IF (BEST_FRATIO .LT. 1.0  .AND.
   +            MODLIST .GT. 1) BEST_MODEL=CONSTANT
            IF (MODEL .NE. BEST_MODEL) THEN
                MODEL  = BEST_MODEL
                CALL DMODEL (VERTEX, B)
                IDF     = IPTS   NUM_B
                WRITE (KOUT,273) MODEL, NUM_B, IPTS
273             FORMAT(/,1X,'MODEL',I4,', using',I3,' out of',I3,
   +                ' degrees-of-freedom, is optimum.',/,1X)
                IF (MODEL .EQ. CONSTANT) WRITE (KOUT,275)
275             FORMAT(1X,'WARNING - Review data carefully.  Failure',
   +                ' to obtain a good fit may be due',/,
   +                11X,'to erronous data.  Look for ',
   +                'unexpected RESIDUAL values.',/,1X)
                MERIT    = AMOEBA0(VERTEX,MFVCT,IBMAX,NUM_B,IBMAX+1,
   +                           CONVERGENCE,MERITF,NUMITR,B,WORK)
            ENDIF
        ENDIF
    ENDIF
    CLOSE (IFILE3,STATUS='DELETE')
    IF (IERR .EQ. NO_ERROR) THEN
        CALL POST
    ENDIF
    IF (IERR .NE. NO_ERROR) THEN
        WRITE (CERR,901) IERR
901     FORMAT(I6)
        CALL LTJUST(CERR)
        OPEN  (IFILE3,FILE='MELT.ERR',STATUS='OLD')
        CALL PARSFILE (INT2(IFILE3),INT2(1),CERR(1:LENSTR(CERR)),
   +                   INT2(2),CATALOG)
        IF (IERR .LT. 200) THEN
            WRITE (KOUT,911) CATALOG(1:LENSTR(CATALOG)), KBELL
911         FORMAT(1X,A,1A1)
        ELSE
            WRITE (KOUT,911) CATALOG(1:LENSTR(CATALOG))
        ENDIF
    ENDIF
    STOP ' '
    END
```

```
      SUBROUTINE PREFIT (VERTEX)
      CHARACTER*4    I1A4
      REAL*8         N_OF_D, N_OF_D_MINUS_OLD_N, DN_BY_DD
      EXTERNAL       N_OF_D, N_OF_D_MINUS_OLD_N, DN_BY_DD
      INTEGER*2      LENSTR
      INTEGER*2      I, J
      INTEGER*4      I4TEMP
      REAL*4         RTEMP
      REAL*4         HMS2HR, HR2HMS
      REAL*8         RAD, DEG, DPTEMP
      REAL*4         SUBIND
      LOGICAL*2      INVALID, FOUND
      CHARACTER*1    BLANK, KBELL, KFF
      CHARACTER*80   I1A80
      PARAMETER      (BLANK = ' ')
$INCLUDE: 'SYMBOLA.FTN'
$INCLUDE: 'SYMBOLB.FTN'
$INCLUDE: 'SYMBOLC.FTN'
$INCLUDE: 'SYMBOLG.FTN'
$INCLUDE: 'COMMONA.FTN'
$INCLUDE: 'COMMONB.FTN'
$INCLUDE: 'COMMONC.FTN'
$INCLUDE: 'COMMONE.FTN'
$INCLUDE: 'COMMONF.FTN'
$INCLUDE: 'COMMONG.FTN'
$INCLUDE: 'COMMONH.FTN'
$INCLUDE: 'COMMONJ.FTN'
      REAL*4       VERTEX
      DIMENSION    VERTEX(IBMAX,IBMAX+1)
      KBELL       = CHAR(7)
      KFF         = CHAR(12)
      PART_NUMBER     = NULL
      PROJECT_NUMBER  = NULL
      GLASS_TYPE      = NULL
      MFGR            = NULL
      SUPPLIER        = NULL
      MELT_NUMBER     = NULL
      ANNEAL_NUMBER   = NULL
      FORM            = NULL
      COMPANY         = BLANK
      CATALOG         = BLANK
      MIN_WVL         = 0.400
      MAX_WVL         = 0.700
      DEFAULT_ERR_BAR= 0.0
      NUM_DESIGN_WVL = 0
      CONVERGENCE     = 1.0E-4
      MODEL           = 4
      MFTYPE          = WEIGHTED_SUM_OF_SQUARED
      IPTS            = 0
      NOM_IPTS        = 0
      NUMMOD          = 0
      OLD_ANGLE       = 0.0
      NEW_ANGLE       = 0.0
      RISK            = 0.05
      LOT_NAME        = NULL
      SHORT           = .FALSE.
      TEMPERATURE     = 0.0
      PRESSURE        = 0.0
      PLOTTER         = .FALSE.
      PLOT_WVL        = .TRUE.
      PLOT_FRQ        = .FALSE.
      FF_END          = .FALSE.
      MODLIST         = 0
      HAVE_HISTORY    = .FALSE.
      UPDATE_HISTORY  = .FALSE.
      FNAME3          = 'HISTORY.MEL'
      FNAME1          = 'MELT.MEL'
      BATCH           = .FALSE.
      CHECK           = .FALSE.
      A0              = 1.D0
      A1              = 1.D-2
      A2              = 1.D-2
      A3              = 1.D-3
      A4              = 1.D-4
      A5              = 1.D-5
      DO 105  I=1, MAXMOD
```

```
        HISTORY(I,1)  = 0
        HISTORY(I,2)  = INT4(I)
105     CONTINUE
    INQUIRE (FILE='MELT.MEL',EXIST=FOUND)
    IF (FOUND) THEN
        IERR        = NO_ERROR
        OPEN (IFILE1,FILE='MELT.MEL',STATUS='OLD')
        CALL USERDATA (IFILE1)
        CLOSE (IFILE1,STATUS='KEEP')
        IF (IERR .NE. NO_ERROR) RETURN
    ENDIF
    IERR        = NO_ERROR
    CALL CMDARG (1, FNAME1, I4TEMP)
    IF (I4TEMP .GT. 0) THEN
        OPEN  (IFILE1,FILE=FNAME1,STATUS='OLD')
        CALL USERDATA (IFILE1)
        CLOSE (IFILE1,STATUS='KEEP')
    ENDIF
    IF (IERR .NE. NO_ERROR) RETURN
    WRITE (KOUT,109)
109 FORMAT(1X)
    IF (.NOT. BATCH) THEN
        CALL USERDATA (KEYB)
        IF (IERR .NE. NO_ERROR) RETURN
        WRITE (KOUT,109)
    ELSE
        IF (CHECK) THEN
            IERR    = QUIT_SPECIFIED
            RETURN
        ENDIF
    ENDIF
    IF (NOM_IPTS .GT. 1) THEN
        CALL SORT2DR4 (NOMINAL, MAX_NOM_IPTS, NOM_IPTS, 2, 2)
    ENDIF
    COMPUTE_EXPN = .FALSE.
    IF (NUM_DESIGN_WVL .GT. 0) THEN
        DO 139  I=1, NUM_DESIGN_WVL
          IF (DESIGN_EXPN(I) .EQ. 0.0) THEN
           IF (NOM_IPTS .GT. 0) THEN
            DO 135  J=1, NOM_IPTS
              IF (ABS(1.0-NOM_WVL(J)/DESIGN_WVL(I)).LT.1e-4) GOTO 136
135           CONTINUE
            COMPUTE_EXPN   = .TRUE.
            GOTO 138
136         DESIGN_EXPN(I) = NOM_EXPN(J)
           ELSE
            COMPUTE_EXPN   = .TRUE.
           ENDIF
          ENDIF
138       CONTINUE
139       CONTINUE
    ENDIF
    DO 149  I=1, IPTS
      IF (EXPN(I) .EQ. 0.0 .AND. NOM_IPTS .GT. 0) THEN
          IF (NOM_IPTS .GT. 0) THEN
            DO 145  J=1, NOM_IPTS
              IF (ABS(1.0-NOM_WVL(J)/WVL(I)) .LT. 1e-4) GOTO 146
145           CONTINUE
            COMPUTE_EXPN   = .TRUE.
            GOTO 148
146         EXPN(I)        = NOM_EXPN(J)
          ELSE
            COMPUTE_EXPN   = .TRUE.
          ENDIF
      ENDIF
148   CONTINUE
149   CONTINUE
    IF (NUM_DESIGN_WVL .GT. 1) THEN
        CALL SORT2DR4 (DESIGN, MAX_DESIGN_WVL, NUM_DESIGN_WVL, 3, 2)
        I        = 1
150     I        = I + 1
        IF (I .LE. NUM_DESIGN_WVL) THEN
            IF (DESIGN_WVL(I) .EQ. DESIGN_WVL(I-1)) THEN
                DO 157  J=I, NUM_DESIGN_WVL
                    DESIGN_WVL(J-1) = DESIGN_WVL(J)
                    DESIGN_EXPN(J-1)= DESIGN_EXPN(J)
```

```
157                 CONTINUE
                  NUM_DESIGN_WVL = NUM_DESIGN_WVL   1
              ENDIF
              GOTO 150
          ENDIF
      ENDIF
      CALL DMODEL (VERTEX, B)
      IF (.NOT. COMPUTE_EXPN) GOTO 400
      IF (MFGR .EQ. BLANK) THEN
          WRITE (KOUT,181) KBELL
181       FORMAT(1X,'WARNING - No manufacturer specified, SCHOTT used.',
     2            1A1)
          MFGR      = 'SCHOTT'
          I1A80     = CATALOG(1:LENSTR(CATALOG)) // 'SCHOTT'
      ELSE
          I1A80     = CATALOG(1:LENSTR(CATALOG)) //  MFGR(1:LENSTR(MFGR))
      ENDIF
      INVALID       = .FALSE.
182   CALL NEWSUF (I1A80,'TXT')
      INQUIRE (FILE=I1A80,EXIST=FOUND)
      IF (FOUND) THEN
          OPEN  (IFILE1,FILE=I1A80,STATUS='OLD')
          IERR        = NO_ERROR
          CALL NOMDAT (IFILE1)
          CLOSE (IFILE1,STATUS='KEEP')
          IF (IERR .NE. NO_ERROR) THEN
              IF (ICOM .EQ. COMPUTE_INDEX_ERROR) RETURN
              IF (ICOM .EQ. COMPUTE_SQUARED_INDEX_ERROR) RETURN
          ELSE
              CALL DMODEL (VERTEX, B)
          ENDIF
      ELSE
          IF (.NOT. INVALID) THEN
              WRITE (KOUT,185) MFGR(1:LENSTR(MFGR))
185           FORMAT(1X,'ERROR - Unrecognized manufacturer (',A,').')
          ENDIF
          WRITE (KOUT,187) I1A80(1:LENSTR(I1A80)), KBELL
187       FORMAT(1X,'ERROR   File not found (',A,1A1,').')
          IF (INVALID) THEN
              IERR        = INVALID_MFGR
              RETURN
          ENDIF
          INVALID     = .TRUE.
          WRITE (KOUT,189)
189       FORMAT(1X,'WARNING - SCHOTT catalog used.')
          MFGR      = 'SCHOTT'
          I1A80     = CATALOG(1:LENSTR(CATALOG)) // 'SCHOTT'
          GOTO 182
      ENDIF
400   DO 409  J=1, IPTS
          IF (IACT(J) .EQ. 1) OBSN(J)=EXPN(J)+OBSN(J)
409       CONTINUE
      CALL SORT2DR4 (EXPERIMENTAL, MAXPTS, IPTS, 4, 4)
      OPEN (IFILE2,STATUS='NEW')
      IF (OLD_ANGLE .NE. 0.0) THEN
          WRITE (KOUT,115) KBELL, OLD_ANGLE, NEW_ANGLE
          WRITE (IFILE2,115) KFF, OLD_ANGLE, NEW_ANGLE
115       FORMAT(1X,1A1,/,1X,'WARNING - The OBSERVED INDEX was ',
     +        'altered to compensate for the change',/,
     +        11X,'in prism angle from',F9.5,' to',F9.5,' degrees '.
     +        '(HMS).',/,/,
     +        1X,'EXPERIMENTAL',T23,'DEVIATION ANGLE',T43,
     +        7('-'),' OBSERVED INDEX ',7('-'),/,
     +        2X,'WAVELENGTH',T22,'RADIANS',T37,'HMS',T48,'NEW',
     +        T59,'OLD',T67,'CHANGE')
          WRITE (KOUT,109)
          WRITE (IFILE2,109)
          DO 129 I=1, IPTS
              RTEMP    = HMS2HR(OLD_ANGLE)
              PRISMA   = RAD(DBLE(RTEMP))
              OLD_N    = DBLE(OBSN(I))
              DPTEMP    = RAD(45.D0)
              CALL DNEWTN  (N_OF_D_MINUS_OLD_N,
     +                      DN_BY_DD,
     +                      DPTEMP,
     +                      1.0D-7,
```

```
     +                    5.0D-7,
     +                    100,
     +                    IERR)
               IF (IERR .EQ. -1) THEN
                   WRITE (KOUT,125)
125                FORMAT(1X,'ERROR   Unable to adjust data for new '.
     +                    'prism angle.')
                   IERR    = MAX_ITER_EXCEEDED
                   CLOSE (IFILE2,STATUS='DELETE')
                   RETURN
               ELSEIF (IERR .EQ. 1) THEN
                   IERR    = NO_ERROR
               ELSEIF (IERR .EQ. 2) THEN
                   IERR    = NO_ERROR
               ENDIF
               PRISMA  = RAD(DBLE(HMS2HR(NEW_ANGLE)))
               OBSN(I) = SNGL(N_OF_D(DPTEMP))
               CALL GETSYM (WVL(I),I1A4)
               WRITE (KOUT,127) WVL(I), I1A4, SNGL(DPTEMP),
     +                          HR2HMS(SNGL(DEG(DPTEMP))),
     +                          OBSN(I), OLD_N, OBSN(I)-SNGL(OLD_N)
               WRITE (IFILE2,127) WVL(I), I1A4, SNGL(DPTEMP),
     +                          HR2HMS(SNGL(DEG(DPTEMP))),
     +                          OBSN(I), OLD_N, OBSN(I)-SNGL(OLD_N)
127            FORMAT(1X,F10.6,1A4,T20,F9.6,T31,F9.5,3(2X,F9.6))
129            CONTINUE
           WRITE (KOUT,109)
           WRITE (IFILE2,109)
       ENDIF
       RTEMP    = DEFAULT_ERR_BAR
       DO 417  I=1, IPTS
           OBSN2(I) = OBSN(I)**2
           IF (OBSN(I) .EQ. 0.0  .OR.  EXPN(I) .EQ. 0.0) THEN
               ERRN(I)  = 0.0
               ERRN2(I) = 0.0
           ELSE
               ERRN(I)  = SUBIND(OBSN(I),EXPN(I))
               ERRN2(I) = OBSN2(I)   EXPN(I)**2
           ENDIF
           IF (ERROR_BAR(I) .EQ. 0.0) ERROR_BAR(I)=DEFAULT_ERR_BAR
           IF (ERROR_BAR(I) .LT. RTEMP) RTEMP=ERROR_BAR(I)
417        CONTINUE
       DO 517  I=1, IPTS
           IF (RTEMP .NE. 0.0) THEN
               WEIGHT(I)  = ERROR_BAR(I)/RTEMP
           ELSE
               WEIGHT(I)  = 1.0
           ENDIF
517        CONTINUE
       RETURN
       END
```

```
      SUBROUTINE POST
      CHARACTER*1 BLANK, IFF
      PARAMETER   (BLANK=' ')
      REAL*4      FITIND, NOMIND
      REAL*4      CINTER
      REAL*4      DELWVL
      REAL*4      TEMP1, TEMP2, TEMP3, TEMP4
      REAL*4      SUBIND
      INTEGER*2   LENSTR
      INTEGER*4   I, J, K
      LOGICAL*2   FOUND
      LOGICAL*4   L4TEMP
$INCLUDE: 'SYMBOLB.FTN'
$INCLUDE: 'SYMBOLC.FTN'
$INCLUDE: 'SYMBOLG.FTN'
$INCLUDE: 'COMMONA.FTN'
$INCLUDE: 'COMMONB.FTN'
$INCLUDE: 'COMMONF.FTN'
$INCLUDE: 'COMMONG.FTN'
$INCLUDE: 'COMMONH.FTN'
$INCLUDE: 'COMMONI.FTN'
      IFF     = CHAR(12)
      WRITE (IFILE2,115) IFF
  115 FORMAT(1X,1A1)
      IF (IMEAN .EQ. 0) THEN
          J       = NUM_B
      ELSE
          J       = NUM_B
      ENDIF
      IF (ICOM .EQ. COMPUTE_INDEX_ERROR) THEN
          CALL ANOVA (IFILE2, J,      IPTS, WVL, ERRN, TERMS, WEIGHT,
     +                RISK, TEMP1, TEMP2, TEMP3, TEMP4, RSQ, SDEV)
      ELSEIF (ICOM .EQ. COMPUTE_SQUARED_INDEX_ERROR) THEN
          CALL ANOVA (IFILE2, J,      IPTS, WVL, ERRN2, TERMS, WEIGHT,
     +                RISK, TEMP1, TEMP2, TEMP3, TEMP4, RSQ, SDEV)
      ELSEIF (ICOM .EQ. COMPUTE_INDEX) THEN
          CALL ANOVA (IFILE2, J,      IPTS, WVL, OBSN, TERMS, WEIGHT,
     +                RISK, TEMP1, TEMP2, TEMP3, TEMP4, RSQ, SDEV)
      ELSE
          CALL ANOVA (IFILE2, J,      IPTS, WVL, OBSN2, TERMS, WEIGHT,
     +                RISK, TEMP1, TEMP2, TEMP3, TEMP4, RSQ, SDEV)
      ENDIF
      DO 239  I=1, IPTS
              COMPUTED(I) = FITIND(WVL(I))
              IF (IERR .NE. NO_ERROR) RETURN
              RESIDUAL(I) = SUBIND(OBSN(I),COMPUTED(I))
  239     CONTINUE
       DO 259  I=1, NUM_DESIGN_WVL
              DESIGN_N(I) = FITIND(DESIGN_WVL(I))
              IF (IERR .NE. NO_ERROR) RETURN
              DESIGN_ERROR_BAR(I) = CINTER(RISK,DESIGN_WVL(I),
     +                                     WVL,SDEV,IPTS,NUM_B)
  259     CONTINUE
      L4TEMP  = SHORT
      IF (SHORT) SHORT=.FALSE.
      REWIND IFILE2
      CALL REPORT (KOUT)
      SHORT   = L4TEMP
      IF (PRINTER) THEN
          WRITE (KOUT,321)
  321     FORMAT(/,1X,'Sending copy to PRINTER device or file . . .')
          REWIND IFILE2
          CALL REPORT (IPRT)
          IF (FF_END) WRITE (IPRT,115) IFF
      ENDIF
      CLOSE (IFILE2,STATUS='DELETE')
      WRITE (KOUT,606) 'MELTHIST.TXT'
      INQUIRE (FILE='MELTHIST.TXT'. EXIST=FOUND)
      IF (FOUND) THEN
          OPEN (IFILE3,FILE='MELTHIST.TXT',STATUS='OLD',ACCESS='APPEND')
      ELSE
          OPEN (IFILE3,FILE='MELTHIST.TXT',STATUS='NEW')
      ENDIF
      WRITE (IFILE3,721) MODEL, FNAME1(1:LENSTR(FNAME1))
  721 FORMAT(I3,2X,A)
      CLOSE (IFILE3,STATUS='KEEP')
```

```
      NUM_INTERP_WVL  = 0
      DELWVL          = (MAX_WVL-MIN_WVL)/FLOAT(INTERP_MAX)
      DO 515 I=1, INTERP_MAX
          J               = NUM_INTERP_WVL + 1
          INTERP_WVL(J)   = MIN_WVL + DELWVL*FLOAT(I-1)
          INTERP_EXPN(J)  = NOMIND(INTERP_WVL(J))
          IF (INTERP_EXPN(J) .GT. 0.0) THEN
              INTERP_OBSN(J)  = FITIND(INTERP_WVL(J))
              INTERP_ERRN(J)  = SUBIND(INTERP_OBSN(J),INTERP_EXPN(J))
              NUM_INTERP_WVL  = NUM_INTERP_WVL + 1
          ENDIF
  515     CONTINUE
      IF (PLOTTER) THEN
          IF (PLOTTER_DEV .EQ. BLANK) THEN
              CALL NEWSUF (FNAME1,'PLT')
              INQUIRE (FILE=FNAME1,EXIST=FOUND)
              IF (FOUND) CALL SYSDEL (FNAME1)
              PLOTTER_DEV  = FNAME1
          ENDIF
          CALL UPCASE (PLOTTER_TYPE)
          CALL UPCASE (PLOTTER_DEV)
          WRITE (KOUT,521) PLOTTER_DEV(1:LENSTR(PLOTTER_DEV)),
     +                     PLOTTER_TYPE
  521     FORMAT(/,1X,'Sending plotter instructions to ',A,' for ',1A8,
     +           '. . .')
          IF (PLOTTER_DEV .EQ. 'LPT2' .OR. PLOTTER_DEV .EQ. 'LPT3') THEN
              OPEN  (IPLOT, FILE=PLOTTER_DEV, STATUS='OLD')
          ELSE
              OPEN  (IPLOT, FILE=PLOTTER_DEV, STATUS='UNKNOWN')
          ENDIF
          IF (PLOT_WVL) CALL PLOT1 (PLOTTER_TYPE)
          IF (PLOT_FRQ) CALL PLOT2 (PLOTTER_TYPE)
          CLOSE (IPLOT,STATUS='KEEP')
      ENDIF
      IF (UPDATE_HISTORY) THEN
          WRITE (KOUT,606) FNAME3(1:LENSTR(FNAME3))
  606     FORMAT(/,1X,'Updating history file ',A,'. . .')
          INQUIRE (FILE=FNAME3, EXIST=FOUND)
          IF (.NOT. HAVE_HISTORY) THEN
              IF (FOUND) THEN
                  OPEN  (IFILE3,FILE=FNAME3,STATUS='OLD')
                  CALL USERDATA (-IFILE3)
                  CLOSE (IFILE3,STATUS='DELETE')
              ENDIF
          ELSE
              IF (FOUND) CALL SYSDEL (FNAME3)
          ENDIF
          HISTORY(MODEL,1)= HISTORY(MODEL,1) + 1
          K       = 0
          DO 619 I=1, MAXMOD
              K       = K + HISTORY(I,1)
  619         CONTINUE
          CALL SORT2D (HISTORY, MAXMOD, MAXMOD, 2, 2)
          OPEN  (IFILE3,FILE=FNAME3,STATUS='NEW')
          WRITE (IFILE3,621) K
  621     FORMAT('BEGIN HISTORY !',I6,' samples',/,
     +           '!MODEL  COUNT PERCENT')
          DO 639  I=MAXMOD, 1, -1
              WRITE (IFILE3,625) (HISTORY(I,J),J=2,1,-1),
     +                           FLOAT(HISTORY(I,1))/FLOAT(K)*100.0
  625         FORMAT(I6,1X,I6,1X,'!',F6.1)
  639         CONTINUE
          WRITE (IFILE3,649)
  649     FORMAT('END HISTORY')
          CLOSE (IFILE3,STATUS='KEEP')
      ENDIF
      RETURN
      END
```

```
      SUBROUTINE USERDATA (KINPAS)
      CHARACTER*1   KBELL, BLANK
      CHARACTER*1   CTRLZ
      PARAMETER     (BLANK=' ')
      CHARACTER*2   I1A2, J1A2
      CHARACTER*3   KEYWORDS, I1A3
      CHARACTER*5   I1A5
      CHARACTER*80  I1A80
      LOGICAL*2     INVALID, DATA_LOOP
      LOGICAL*2     NOMINAL_LOOP
      LOGICAL*2     FORMULAS_LOOP
      LOGICAL*2     HISTORY_LOOP
      LOGICAL*2     FOUND
      INTEGER*2     I, MAX_KEYWORDS, USERKEY, J, K, K1, K2
      INTEGER*2     LENSTR
      INTEGER*4     KIN, KINOLD, KINPAS
      INTEGER*2     IRTN, J_LOOP, J_LIMIT
      REAL*8        DPREAL
      PARAMETER    (MAX_KEYWORDS=40)
      DIMENSION     KEYWORDS(MAX_KEYWORDS), USERKEY(MAX_KEYWORDS)
$INCLUDE: 'SYMBOLB.FTN'
$INCLUDE: 'SYMBOLG.FTN'
$INCLUDE: 'COMMONA.FTN'
$INCLUDE: 'COMMONB.FTN'
$INCLUDE: 'COMMOND.FTN'
$INCLUDE: 'COMMONE.FTN'
$INCLUDE: 'COMMONF.FTN'
$INCLUDE: 'COMMONG.FTN'
$INCLUDE: 'COMMONH.FTN'
      DATA KEYWORDS / 'PAR', 'PRO', 'GLA', 'MAN', 'MFG', 'MEL', 'ANN',
     2                'WVL', 'WAV', 'BEG', 'END', 'MAX', 'MIN', 'SUP',
     3                'VEN', 'UNC', 'ERR', 'COM', 'FOR', 'DES', 'IND',
     4                'REA', 'CAT', 'PLO', 'DEB', 'CON', 'MFT', 'MOD',
     5                'PRI', 'ANG', 'RIS', 'LOT', 'SHO', 'GO ', 'QUI',
     6                'TEM', 'PRE', 'FFE', 'HIS', 'BAT'                /
      DATA USERKEY  /     1,     2,     3,     4,     4,     5,     6,
     2                   -8,    -8,    -1,    -2,   102,   101,     7,
     3                    7,   103,   103,    -3,     8,    -8,    -9,
     4                   -4,    -5,    -6,    -7,   104,   -10,   -11,
     5                  -12,   205,   107,     9,   -13,   -14,   -15,
     6                  108,   109,   -16,   -17,   -18               /
      KBELL           = CHAR(7)
      CTRLZ           = CHAR(26)
      KIN             = IABS(KINPAS)
      KINOLD          = -1
      DATA_LOOP       = .FALSE.
      COMPUTE_EXPN    = .FALSE.
      FORMULAS_LOOP   = .FALSE.
      HISTORY_LOOP    = .FALSE.
  100 IF (KIN .EQ. KEYB) CALL NOCRLF (' MEL> ')
      READ  (KIN,101,END=300) I1A80
  101 FORMAT(1A80)
      J           = INDEX(I1A80,CTRLZ)
      IF (J .EQ. 1) THEN
          GOTO 300
      ELSEIF (J .GT. 1) THEN
          I1A80   = I1A80(1:J-1)
      ENDIF
      K           = LENSTR(I1A80)
      IF (KIN .NE. KEYB .AND. KINPAS .GE. 0) THEN
          IF (K .GT. 0) THEN
              WRITE (KOUT,103) I1A80(1:K)
  103         FORMAT(1X,A)
          ELSE
              WRITE (KOUT,103)
          ENDIF
      ENDIF
      K           = INDEX(I1A80,'!')
      IF (K .GT. 1) THEN
          I1A80     = I1A80(1:K-1)
      ELSEIF (K .EQ. 1) THEN
          GOTO 100
      ENDIF
      CALL PARSEC (1, I1A80, BLANK, I1A3)
      IF (I1A3 .EQ. BLANK) GOTO 100
      CALL UPCASE (I1A3)
```

```
      DO 119  I=1, MAX_KEYWORDS
          IF (I1A3 .EQ. KEYWORDS(I)) GOTO 130
119       CONTINUE
      IF (DATA_LOOP)      GOTO 400
      IF (NOMINAL_LOOP)   GOTO 500
      IF (FORMULAS_LOOP)  GOTO 600
      IF (HISTORY_LOOP)   GOTO 700
      WRITE (KOUT,121) I1A3, KBELL
121   FORMAT(1X,'WARNING - Unrecognized keyword (',1A3,1A1,'), entire ',
     2       'line disgarded.')
      GOTO 100
130   IF (USERKEY(I) .LT. 0) THEN
          IF (USERKEY(I) .EQ. -1) THEN
              CALL PARSEC (2, I1A80, 'DAT', I1A3)
              CALL UPCASE (I1A3)
              IF (I1A3 .EQ. 'DAT') THEN
                  DATA_LOOP    = .TRUE.
              ELSEIF (I1A3 .EQ. 'NOM') THEN
                  NOMINAL_LOOP= .TRUE.
              ELSEIF (I1A3 .EQ. 'FOR') THEN
                  FORMULAS_LOOP= .TRUE.
              ELSEIF (I1A3 .EQ. 'HIS') THEN
                  HISTORY_LOOP = .TRUE.
              ELSE
                  WRITE (KOUT,137) I1A3, KBELL
137               FORMAT(1X,'WARNING - Unrecognized qualifier (',1A3,
     2                   1A1,'. entire line disgarded.')
              ENDIF
          ELSEIF (USERKEY(I) .EQ. -2) THEN
              CALL PARSEC (2, I1A80, BLANK, I1A3)
              CALL UPCASE (I1A3)
              IF (I1A3 .EQ. BLANK .AND. DATA_LOOP)      I1A3='DAT'
              IF (I1A3 .EQ. BLANK .AND. NOMINAL_LOOP)   I1A3='NOM'
              IF (I1A3 .EQ. BLANK .AND. FORMULAS_LOOP)  I1A3='FOR'
              IF (I1A3 .EQ. BLANK .AND. HISTORY_LOOP)   I1A3='HIS'
              IF (I1A3 .EQ. 'DAT') THEN
                  DATA_LOOP    = .FALSE.
              ELSEIF (I1A3 .EQ. 'NOM') THEN
                  NOMINAL_LOOP= .FALSE.
              ELSEIF (I1A3 .EQ. 'FOR') THEN
                  FORMULAS_LOOP= .FALSE.
              ELSEIF (I1A3 .EQ. 'HIS') THEN
                  HISTORY_LOOP = .FALSE.
              ELSEIF (I1A3 .EQ. BLANK) THEN
                  GOTO 300
              ELSE
                  WRITE (KOUT,137) I1A3, KBELL
              ENDIF
          ELSEIF (USERKEY(I) .EQ. -3) THEN
              CALL PARSEC (2, I1A80, BLANK, COMPANY)
          ELSEIF (USERKEY(I) .EQ. -4) THEN
              K1           = 1
              CALL PARSEC (2, I1A80, BLANK, I1A80)
              FNAME2       = I1A80
152           IF (FNAME2 .NE. BLANK) THEN
                  INQUIRE (FILE=FNAME2,EXIST=FOUND)
                  IF (FOUND) THEN
                      IF (KIN .NE. IFILE2) THEN
                          KINOLD     = KIN
                          KIN        = IFILE2
                          OPEN (KIN,FILE=FNAME2,STATUS='OLD')
                      ELSE
                          WRITE (KOUT,155) KBELL
155                       FORMAT(1X,'WARNING - Unable to nest READ ',
     +                          'statements.  Entire line disgarded.',
     +                          1A1)
                      ENDIF
                  ELSE
156                   K1       = K1 + 1
                      IF (K1 .EQ. 2) THEN
                          IF (CATALOG .EQ. BLANK) GOTO 156
                          FNAME2      = CATALOG(1:LENSTR(CATALOG)) //
     +                                  I1A80(1:LENSTR(I1A80))
                      ELSEIF (K1 .EQ. 3) THEN
                          FNAME2      = I1A80
                          CALL NEWSUF (FNAME2,'MEL')
```

```
                    ELSEIF (K1 .EQ. 4) THEN
                        FNAME2      = CATALOG(1:LENSTR(CATALOG)) //
     +                                I1A80(1:LENSTR(I1A80))
                        CALL NEWSUF (FNAME2,'MEL')
                    ELSE
                        WRITE (KOUT,157) I1A80(1:LENSTR(I1A80)), KBELL
157                     FORMAT(1X,'ERROR - File not found (',A,1A1,
     2                         ').')
                        IERR        = FILE_NOT_FOUND
                        RETURN
                    ENDIF
                    WRITE (KOUT,1571) FNAME2(1:LENSTR(FNAME2))
1571                FORMAT(1X,'WARNING   Not found.  Trying READ ',A)
                    GOTO 152
                ENDIF
            ELSE
                WRITE (KOUT,159) KBELL
 159            FORMAT(1X,'WARNING - Filename not specified, entire ',
     2                 'line disgarded.',1A1)
            ENDIF
        ELSEIF (USERKEY(I) .EQ. -5) THEN
            CALL PARSEC (2, I1A80, BLANK, CATALOG)
        ELSEIF (USERKEY(I) .EQ. -6) THEN
            CALL PARSEC (2, I1A80, BLANK, I1A3)
            CALL UPCASE (I1A3)
            IF (I1A3 .EQ. 'OFF') THEN
                PLOTTER = .FALSE.
            ELSEIF (I1A3 .EQ. 'ON') THEN
                PLOTTER = .TRUE.
                CALL PARSEC (3, I1A80, BLANK, PLOTTER_TYPE)
                CALL PARSEC (4, I1A80, BLANK, PLOTTER_DEV)
            ELSE
                PLOT_WVL    = .FALSE.
                PLOT_FRQ    = .FALSE.
                IF (I1A3(1:1) .EQ. 'W') PLOT_WVL=.TRUE.
                IF (I1A3(1:1) .EQ. 'F') PLOT_FRQ=.TRUE.
                CALL PARSEC (3, I1A80, BLANK, I1A3)
                CALL UPCASE (I1A3)
                IF (I1A3(1:1) .EQ. 'W') PLOT_WVL=.TRUE.
                IF (I1A3(1:1) .EQ. 'F') PLOT_FRQ=.TRUE.
            ENDIF
        ELSEIF (USERKEY(I) .EQ. -7) THEN
            CALL PARSEC (2, I1A80, 'NO', I1A2)
            CALL UPCASE (I1A2)
            DEBUG   = .FALSE.
            IF (I1A2(1:1) .EQ. 'Y') DEBUG=.TRUE.
            IF (I1A2(1:1) .EQ. 'T') DEBUG=.TRUE.
        ELSEIF (USERKEY(I) .EQ. -8) THEN
            DO 187  J=1, MAX_DESIGN_WVL-NUM_DESIGN_WVL
                CALL PARSER (J+1, I1A80, 0.D0, DPREAL, INVALID)
                IF (INVALID) THEN
                    CALL PARSEC (J+1, I1A80, BLANK, I1A2)
                    DO 183  K=1, MAX_LINES
                        IF (I1A2.EQ.SPECTRAL_LINE_NAMES(K)) GOTO 186
 183                    CONTINUE
                    WRITE (KOUT,185) I1A2, KBELL
 185                FORMAT(/,1X,'WARNING - Unrecognized symbolic ',
     +                     'wavelength specification (',1A2,1A1,
     +                     '), remainder of line disgarded.')
                    GOTO 100
 186                DPREAL      = DBLE(SPECTRAL_LINE_VALUES(K))
                ENDIF
                IF (DPREAL .LE. 0.D0) GOTO 190
                NUM_DESIGN_WVL = NUM_DESIGN_WVL + 1
                DESIGN_WVL(NUM_DESIGN_WVL) = SNGL(DPREAL)
 187            CONTINUE
        ELSEIF (USERKEY(I) .EQ.  -9) THEN
            DO 1087 J=1, MAX_DESIGN_OBSN-NUM_DESIGN_OBSN
                CALL PARSER (J+1, I1A80, 0.D0, DPREAL, INVALID)
                IF (INVALID) GOTO 900
                K           = USERKEY(I) - USERKEY(I)/100*100 +
     2                        NUM_DESIGN_OBSN
                IF (DPREAL .LE. 0.D0) GOTO 190
                NUM_DESIGN_OBSN = NUM_DESIGN_OBSN + 1
                DESIGN_EXPN(NUM_DESIGN_OBSN) = SNGL(DPREAL)
1087            CONTINUE
```

```
      ELSEIF (USERKEY(I) .EQ. -10) THEN
          CALL PARSER (2, I1A80, 1.D0, DPREAL, INVALID)
          IF (INVALID) GOTO 900
          MFTYPE  = IFIX(SNGL(DPREAL))
      ELSEIF (USERKEY(I) .EQ. -11) THEN
          K       = 2
1088      CONTINUE
              CALL PARSER (INT4(K), I1A80, -999.D0, DPREAL, INVALID)
              IF (INVALID) GOTO 900
              J       = IFIX(SNGL(DPREAL))
              IF  (J .EQ. 0 .OR. (J .EQ. -999 .AND. K .EQ. 2)) THEN
                  CLOSE (IFILE3,STATUS='DELETE')
                  OPEN  (IFILE3,FORM='UNFORMATTED',STATUS='NEW')
                  MODLIST = 0
              ELSEIF (J .EQ. -999) THEN
                  GOTO 190
              ELSE
                  IF ((J .LT. 0)  .OR.  (J .GT. MAXMOD)) THEN
                      IERR    = ILLEGAL_MODEL_NUMBER
                      RETURN
                  ELSE
                      MODLIST = MODLIST + 1
                      MODEL   = INT4(J)
                      WRITE (IFILE3) MODEL
                  ENDIF
              ENDIF
              K       = K + 1
              GOTO 1088
      ELSEIF (USERKEY(I) .EQ. -12) THEN
          CALL PARSEC (2, I1A80, BLANK, I1A3)
          CALL UPCASE (I1A3)
          IF (I1A3 .EQ. 'OFF') THEN
              IF (PRINTER) CLOSE (IPRT)
              PRINTER     = .FALSE.
          ELSEIF (I1A3 .EQ. 'ON') THEN
              IF (PRINTER) CLOSE (IPRT)
              CALL PARSEC (3, I1A80, BLANK, I1A80)
              CALL UPCASE (I1A80)
              IF (I1A80 .EQ. 'LPT2' .OR. I1A80 .EQ. 'LPT3') THEN
                  OPEN  (IPRT, FILE=I1A80, STATUS='OLD')
              ELSE
                  OPEN  (IPRT, FILE=I1A80, STATUS='UNKNOWN')
              ENDIF
              PRINTER     = .TRUE.
          ELSE
              WRITE (KOUT,137) I1A3, KBELL
          ENDIF
      ELSEIF (USERKEY(I) .EQ. -13) THEN
          CALL PARSEC (2, I1A80, 'YES', I1A2)
          CALL UPCASE (I1A2)
          SHORT   = .FALSE.
          IF (I1A2(1:1) .EQ. 'Y') SHORT=.TRUE.
          IF (I1A2(1:1) .EQ. 'T') SHORT=.TRUE.
      ELSEIF (USERKEY(I) .EQ. -14) THEN
          GOTO 300
      ELSEIF (USERKEY(I) .EQ. -15) THEN
          IERR    = QUIT_SPECIFIED
          RETURN
      ELSEIF (USERKEY(I) .EQ. -16) THEN
          CALL PARSEC (2, I1A80, 'YES', I1A2)
          CALL UPCASE (I1A2)
          FF_END  = .FALSE.
          IF (I1A2(1:1) .EQ. 'Y') FF_END=.TRUE.
          IF (I1A2(1:1) .EQ. 'T') FF_END=.TRUE.
      ELSEIF (USERKEY(I) .EQ. -17) THEN
          CALL PARSEC (2, I1A80, 'YES', I1A2)
          CALL UPCASE (I1A2)
          IF (I1A2(1:1) .EQ. 'Y' .OR. I1A2(1:1) .EQ. 'T') THEN
              UPDATE_HISTORY  = .TRUE.
          ELSEIF (I1A2(1:1) .EQ. 'F') THEN
              CALL PARSEC (3, I1A80, FNAME3, FNAME3)
          ELSE
              UPDATE_HISTORY  = .FALSE.
          ENDIF
      ELSEIF (USERKEY(I) .EQ. -18) THEN
          CALL PARSEC (2, I1A80, 'YES', I1A2)
```

```
            CALL UPCASE (I1A2)
            BATCH   = .FALSE.
            CHECK   = .FALSE.
            IF (I1A2(1:1) .EQ. 'Y') BATCH=.TRUE.
            IF (I1A2(1:1) .EQ. 'T') BATCH=.TRUE.
            IF (I1A2(1:1) .EQ. 'C') THEN
                BATCH   = .TRUE.
                CHECK   = .TRUE.
            ENDIF
        ENDIF
    ELSEIF (USERKEY(I) .LE. 100) THEN
        CALL PARSEC (2, I1A80, BLANK, USERCHAR(USERKEY(I)))
    ELSEIF (USERKEY(I) .GT. 100) THEN
        DO 195  K=1, USERKEY(I)/100
            CALL PARSER (K+1, I1A80, 0.D0, DPREAL, INVALID)
            IF (INVALID) GOTO 900
            J           = USERKEY(I)   USERKEY(I)/100*100 + K - 1
            USERREAL(J) = SNGL(DPREAL)
195         CONTINUE
190 ENDIF
    GOTO 100
300 IF (KIN .EQ. IFILE2) THEN
        CLOSE (KIN,STATUS='KEEP')
        KIN      = KINOLD
        KINOLD   = -1
        GOTO 100
    ENDIF
    RETURN
400 J_LOOP    = IPTS
    J_LIMIT   = MAXPTS
    ASSIGN 410 TO IRTN
    GOTO 420
410 IPTS      = J_LOOP
    GOTO 100
420 IF (J_LOOP .LT. J_LIMIT) THEN
        J         = J_LOOP + 1
        IF (DATA_LOOP) THEN
        CALL PARSER (4, I1A80, 0.D0, DPREAL, INVALID)
        IF (.NOT. INVALID) EXPN(J) = SNGL(DPREAL)
        CALL PARSER (3, I1A80, 0.D0, DPREAL, INVALID)
        IF (.NOT. INVALID) ERROR_BAR(J) = SNGL(DPREAL)
        ENDIF
        CALL PARSER (2, I1A80, 0.D0, DPREAL, INVALID)
        IF (INVALID) GOTO 900
        IF (DATA_LOOP) THEN
            OBSN(J)     = SNGL(DPREAL)
            IACT(J)     = 0
        ENDIF
        IF (NOMINAL_LOOP) NOM_EXPN(J) = SNGL(DPREAL)
        CALL PARSER (1, I1A80, 0.D0, DPREAL, INVALID)
        IF (INVALID) THEN
            CALL PARSEC (1, I1A80, BLANK, I1A5)
            K         = INDEX(I1A5,'-')
            IF (K .GT. 0) THEN
                I1A2      = I1A5(1:K-1)
                J1A2      = I1A5(K+1:LENSTR(I1A5))
                DO 423   K=1, MAX_LINES
                    IF (I1A2 .EQ. SPECTRAL_LINE_NAMES(K)) GOTO 428
423                 CONTINUE
                WRITE (KOUT,185) I1A2, KBELL
                GOTO IRTN
428             K1        = K
                DO 433   K=1, MAX_LINES
                    IF (J1A2 .EQ. SPECTRAL_LINE_NAMES(K)) GOTO 438
433                 CONTINUE
                WRITE (KOUT,185) J1A2, KBELL
                GOTO IRTN
438             K2        = K
                IF (DATA_LOOP .AND. K1 .NE. K2) THEN
                DO 443   K=1, J_LOOP
                    IF (ABS(1.0-WVL(K)/SPECTRAL_LINE_VALUES(K1))
  2                                                 .LE. 0.005) THEN
                        WVL(J)    = SPECTRAL_LINE_VALUES(K2)
                        OBSN(J)   = OBSN(K) - OBSN(J)
                        IF (EXPN(J) .NE. 0.0) EXPN(J)=EXPN(K)-EXPN(J)
                        GOTO 448
```

```
                    ELSEIF (ABS(1.0-WVL(K)/SPECTRAL_LINE_VALUES(K2))
     2                                                    .LE. 0.005) THEN
                        WVL(J)    = SPECTRAL_LINE_VALUES(K1)
                        OBSN(J)   = OBSN(K) + OBSN(J)
                        IF (EXPN(J) .NE. 0.0) EXPN(J)=EXPN(K)+EXPN(J)
                        GOTO 448
                    ENDIF
 443                CONTINUE
                ELSEIF (DATA_LOOP .AND. K1 .EQ. K2) THEN
                    WVL(J)  = SPECTRAL_LINE_VALUES(K1)
                    IACT(J) = 1
                    GOTO 548
                ELSEIF (NOMINAL_LOOP) THEN
                DO 543   K=1, J_LOOP
                    IF (ABS(1.0-NOM_WVL(K)/SPECTRAL_LINE_VALUES(K1))
     2                                                    .LE. 0.005) THEN
                        NOM_WVL(J)    = SPECTRAL_LINE_VALUES(K2)
                        NOM_EXPN(J)   = NOM_EXPN(K) - NOM_EXPN(J)
                        GOTO 548
                    ELSEIF (ABS(1.0-NOM_WVL(K)/
     2                         SPECTRAL_LINE_VALUES(K2)) .LE. 0.005) THEN
                        NOM_WVL(J)    = SPECTRAL_LINE_VALUES(K1)
                        NOM_EXPN(J)   = NOM_EXPN(K) + NOM_EXPN(J)
                        GOTO 548
                    ENDIF
 543                CONTINUE
                ENDIF
                WRITE (KOUT,445) KBELL
 445            FORMAT(1X,'WARNING - Neither symbolic wavelength ',
     2                 'specified previously, entire line ',
     3                 'disgarded.',1A1)
                GOTO IRTN
 448             IF (EXPN(J) .NE. 0.0 .AND. COMPUTE_EXPN) THEN
                    WRITE (KOUT,449) KBELL
 449                FORMAT(1X,'WARNING   Unable to evaluate user-',
     2                     'specified expected index differences ',
     3                     /,1X,'since some previous entries do not',
     4                     ' have expected index specified.',1A1)
                    GOTO IRTN
                ENDIF
 548            CONTINUE
            ELSE
                I1A2      = I1A5(1:2)
                DO 473   K=1, MAX_LINES
                    IF (I1A2 .EQ. SPECTRAL_LINE_NAMES(K)) GOTO 478
 473                CONTINUE
                WRITE (KOUT,185) I1A2, KBELL
                GOTO IRTN
 478            IF (DATA_LOOP)     WVL(J)     = SPECTRAL_LINE_VALUES(K)
                IF (NOMINAL_LOOP) NOM_WVL(J) = SPECTRAL_LINE_VALUES(K)
            ENDIF
        ELSE
            IF (DATA_LOOP)     WVL(J)     = SNGL(DPREAL)
            IF (NOMINAL_LOOP) NOM_WVL(J) = SNGL(DPREAL)
        ENDIF
        IF (DATA_LOOP .AND. EXPN(J) .EQ. 0.0) COMPUTE_EXPN = .TRUE.
        J_LOOP    = J
    ELSE
        WRITE (KOUT,491) J_LIMIT, KBELL
 491    FORMAT(1X,'WARNING - Array dimensions exceeded,',I3,1A1,
   2           'points maximum.  Entire line disgarded.')
    ENDIF
    GOTO IRTN
 500 J_LOOP    = NOM_IPTS
    J_LIMIT   = MAX_NOM_IPTS
    ASSIGN 510 TO IRTN
    GOTO 420
 510 NOM_IPTS  = J_LOOP
    GOTO 100
 600 J       = NUMMOD + 1
    CALL PARSER (1, I1A80, 0.D0, DPREAL, INVALID)
    IF (INVALID) GOTO 900
    K       = IFIX(SNGL(DPREAL))
    IF (K .GT. 0  .AND.  K .LE. MAXMOD) THEN
        NUMMOD     = J
        MODTAG(J)  = K
```

```
        CALL PARSEC (-2, I1A80, BLANK, FORMULAS(K))
    ELSE
        IERR        = ILLEGAL_MODEL_NUMBER
    ENDIF
    GOTO 100
700 CALL PARSER (1, I1A80, 0.D0, DPREAL, INVALID)
    IF (INVALID) GOTO 900
    J       = IFIX(SNGL(DPREAL))
    IF (J .GT. 0  .AND.  J .LE. MAXMOD) THEN
        CALL PARSER (2, I1A80, 0.D0, DPREAL, INVALID)
        IF (INVALID) GOTO 900
        K           = IFIX(SNGL(DPREAL))
        HISTORY(J,1)= INT4(K)
        HISTORY(J,2)= INT4(J)
        HAVE_HISTORY= .TRUE.
    ELSE
        IERR        = ILLEGAL_MODEL_NUMBER
        RETURN
    ENDIF
    GOTO 100
900 WRITE (KOUT,901) KBELL
901 FORMAT(/,1X,'WARNING - Real-valued token expected, unable to '.
   2       'parse.',1A1)
    GOTO 100
    END
```

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• References

1. Schott Optical Glass, Optical Glass Catalogue, Duryea, PA (1980).

2. Ohara Optical Glass Manufacturing Co., Optical Glass Catalogue, Sagimihara, Japan (1980).

3. Hoya Corporation, Optical Glass Catalogue, Tokyo, Japan (1980).

4. Corning-France, Optical Glass Catalogue, Avon, France (1980).

5. Chance Pilkington, Optical Glass Catalog, St. Asaph, Clwyd, U.K. (1980).

6. Malitson, I.H., *Interspecimen Comparison of the Refractive Index of fused Silica*, J. Opt. Soc. Am., 55, 1205 (1965).

7. P. N. Robb, *Selection of Optical Glasses 1: Two Materials*, Appl. Opt., 24, 1864 (1985).

8. M. T. Houk, *Theory, Fabrication, and Testing of Gradients in Flouride Materials*, Ph.D Thesis Proposal, University of Rochester, Institute of Optics (1986).

9. M. Herzberger, *Refractive Indices of Infrared Optical Materials and Color Correction of Infrared Lenses*, J. Opt. Soc. Am., 52, 420 (1962).

10. G. W. Forbes, *Weighted Truncation of Power Series and the Computation of Chromatic Aberration Coefficients*, J. Opt. Soc. Am. A, 1, 350 (1984).

11. H. A. Buchdahl, Optical Aberration Coefficients, (Cambridge, Dover, 1968), pp. 151-152.

12. P. N. Robb and R. I. Mercado, *Calculation of Refractive Indices using Buchdahl's Chromatic Coordinate*, Appl. Opt., 22, 1198 (1983).

13. Schott, p. 6 (reference 1).

14. Robb & Mercado, p. 1198 (reference 12).

15. J. R. Rice, Numerical Methods, Software, and Analysis, (McGraw-Hill, NY, 1983), pp. 108-112.

16. Robb & Mercado, p. 1199 (reference 12).

17. R. Kingslake, Lens Design Fundamentals, (Academic Press, NY, 1978), pp. 12-14.

18. Kingslake, pp. 12-14 (reference 17).

19. B. W. Morrissey & C. J. Powell, *Interpolation of Refractive Index Data*, Appl. Opt., 12, 1588 (1973).

20. W. J. Smith, Modern Optical Engineering, (McGraw-Hill, NY, 1966), pp. 147-148.

21. Smith, pp. 147-148 (reference 20).

22. R. W. Ditchburn, Light, (Interscience Publishers, NY, 1953), pp. 452-456.

23. L. E. Sutton & O. N. Stavroudis, *Fitting Refractive Index Data by Least-Squares*, J. Opt. Soc. Am., 22, 901 (1961).

24. M. Born & E. Wolf, Principles of Optics, (Pergamon Press, Oxford, 1980), pp. 92-98.

25. Smith, p. 148 (reference 20).

26. Kingslake, pp. 12-14 (reference 17).

27. Kingslake, pp. 12-14 (reference 17).

28. M. Herzberger, *Colour Correction in Optical Systems and a New Dispersion Formula*, Optical Acta, 6, 197 (1959).

29. Herzberger, p. 420 (reference 9).

30. Born & Wolf, p. 92 (reference 24).

31. G. W. Forbes, *Chromatic Coordinates in Aberration Theory*, J. Opt. Soc. Am. A, 1, 344 (1984).

32. F. A. Jenkins & H. E. White, Fundamentals of Optics, (McGraw-Hill, 1976), pp. 482-487.

33. M. Herzberger, Modern Geometrical Optics, (Interscience Publishers, NY, 1958), pp. 121-122.

34. Herzberger, p. 197 (reference 28).

35. Schott, p. 36 (reference 1).

36. Ditchburn, pp. 452-456 (reference 22).

37. Ditchburn, pp. 452-456 (reference 22).

38. Ditchburn, pp. 452-456 (reference 22).

39. Born & Wolf, pp. 91-97 (reference 24).

40. Sutton & Stavroudis, p. 901 (reference 23).

41. Sutton & Stavroudis, p. 901 (reference 23).

42. Born & Wolf, pp. 91-97 (reference 24).

43. I. H. Malitson, G. W. Cleek, O. N. Stavroudis, and L. E. Sutton, *Infrared Dispersion of Some Oxide Glasses*, App. Opt., 2, 743 (1963).

44. O. N. Stavroudis & L. E. Sutton, *Rapid Method of Interpolating Refractive Index Measurements*, J. Opt. Soc. Am., 51, 368 (1961).

45. Smith, pp. 147-148 (reference 20).

46. Kingslake, pp. 12-14 (reference 17).

47. Kingslake, p. 13 (reference 17).

48. Smith, p. 148 (reference 20).

49. Herzberger, p. 121 (reference 33).

50. Herzberger, p. 420 (reference 9).

51. R.D. Geiser, *Precision and Accuracy*, Applied Optics and Optical Engineering, R. Kingslake, ed., (Academic Press, 1965), pp. 389-409.

52. D. Stephenson, *Modeling Variation in the Refractive Index of Optical Glasses*, M.S. Thesis Proposal, Rochester Institute of Technology, Center for Imaging Science (1987).

53. Walter G. Driscoll (ed.), Handbook of Optics, (McGraw-Hill 1978), p. 11-1.

54. Robert C. Weast (ed.), CRC Handbook of Chemistry and Physics, (CRC Press 1984), pp. E-189 through E-308.

55. J. A. Nelder & R. Mead, *Computer Journal*, Vol. 7 (1965), p. 308.

56. William H. Press, Numerical Recipes, (Cambridge University Press 1986), pp. 289-293.

57. M. S. Caceci & W. P. Cacheris, *Fitting Curves to Data*, Byte, 340 (May 1984).

58. D. M. Olsson & L. S. Nelson, *The Nelder-Mead Simplex Procedure for Function Minimization*, Technometrics, 17, no. 1, 45 (1975).

59. R. S. Longhurst, Geometrical and Physical Optics, (Wiley & Sons 1967), pp. 86-87.

60. Longhurst, pp. 84-85 (reference 59).

61. Ohara Corporation, *Refractive Index Measurements in Ohara*, internal memo (March 4, 1988).

62. Masumura-san, Ohara Corporation (Japan), personal communication (1990).

63. R. Kingslake (ed), Applied Optics and Optical Engineering, (Academic Press 1969), vol. 5 pp. 3-6.

64. Longhurst, pp. 72-72 (reference 59).

65. Longhurst, pp. 85-86 (reference 59).

66. Longhurst, p. 85 (reference 59).

67. L.W. Tilton, *Prism Refractometry and Certain Goniometrical Requirements for Precision*, Bureau of Standards Journal of Research, 2, 919 (1929).

68. Kingslake, pp. 3-6 (reference 63).

69. Tilton, pp. 909-930 (reference 67).

70. L. W. Tilton, *Prism Size and Orientation in Minimum-Deviation Refractometry*, Bureau of Standards Journal of Research, 6, 59 (1931).

71. L.W. Tilton, *Permissible Curvature of Prism Surfaces and Inaccuracy of Collimation in Precise Minimum-Deviation Refractometry*, Bureau of Standards Journal of Research, 11, 25 (1933).

72. Tilton, p. 25 (reference 71).

73. Longhurst, pp. 82-83 (reference 59).

74. Tilton, p. 924 (reference 67).

75. Tilton, p. 924 (reference 67).

76. D.M. Bates, Nonlinear Regression Analysis and its Applications, (Wiley & Sons 1988), p. 107.

77. Rickmers, pp. 155, 172 (reference 93).

78. Press, p. 165 (reference 56).

79. Press, pp. 503, 506 (reference 56).

80. P.S. Brockington, Ohara Corporation (USA), personal communication (1989).

81. Schott, pp. 36-37, fig. 15-16 (reference 1).

82. Walter Mackintosh, Gaertner Scientific Company, personal communication (1988).

83. Tilton, p. 924 (reference 67).

84. Longhurst, p. 82 (reference 59).

85. G.E. Fishter, *Refractometry*, Applied Optics and Optical Engineering, Volume IV, R. Kingslake [ed.], (Academic Press 1967), pp. 363-367.

86. Smith, pp. 425-426 (reference 20).

87. E. Hecht & A. Zajac, Optics, (Addison-Wesley 1979), pp. 336-337.

88. Smith, p. 392 (reference 20).

89. Smith, p. 392 (reference 20).

90. D. Tentori, J.R. Lerma, *Refractometry by Minimum Deviation: Accuracy Analysis*, Opt. Eng. 29(2), 160-168 (1990).

91. C.F. Gerald, Applied Numerical Analysis, (Addison-Wesley 1980), pp. 8-14.

92. R.J. Nelson et al., *PPC ROM User's Manual*, Privately published by PPC, Santa Ana CA, second edition (1982).

93. A. D. Rickmers, Statistics, An Introduction, (McGraw-Hill 1967), pp. 258-259.

94. Bates, pp. 2-21 (reference 76).

95. Press, p. 59 & 54 (reference 56).

96. Press, p. 52 (reference 56).

97. Press, p. 517 (reference 56).

98. Press (reference 56); Fortran, C, or Pascal versions are availiable.