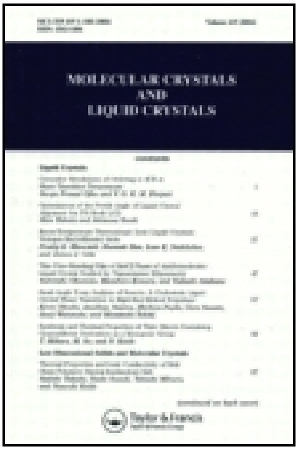

Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl17

A Simple Method to Estimate and Optimize the Optical Slope of TN-Cells and Its Comparison with Experimental Results

Ulrich Finkenzeller [a] & Georg Weber [a]
[a] E. Merck, Industrial Chemicals Division, Frankfurter Straße 250, D 61 Darmstadt, West Germany
Version of record first published: 13 Dec 2006.

Mol. Cryst. Liq. Cryst., 1988, Vol. 164, pp. 145–156
Reprints available directly from the publisher
Photocopying permitted by license only

Printed in the United States of America

A Simple Method to Estimate and Optimize the Optical Slope of TN-Cells and Its Comparison with Experimental Results

ULRICH FINKENZELLER and GEORG WEBER

E. Merck, Industrial Chemicals Division, Frankfurter Straße 250, D 61 Darmstadt, West Germany

(*Received August 27, 1987; in final form March 7, 1988*)

It is shown that the initial slope of the mid-plane tilt angle of a nematic TN-cell correlates well with the associated optical slope for a given cell. Upon determination of the mid-plane tilt angle from the physical parameters of the liquid crystal and the cell-specific correlation coefficients it is easily possible to estimate the optical slope for any material. Cell performance can be optimized qualitatively in terms of the elastic constants, the dielectric anisotropy, and the twist angle.

Keywords: nematic liquid crystals, twisted nematic cell, optical slope, elastic constants, dielectric permittivity

I. INTRODUCTION

The optical slope of a nematic liquid crystalline mixture in a cell is an important property characterizing the optical performance of the display. Today, various theoretical and experimental methods have been established to provide an estimate of the quantity in question.

The chosen approaches range from elaborate theoretical calculations to direct measurements in various experimental set-ups. Examples of the former are the algorithms of Berreman[3] which take into account the physical and optical properties of the liquid crystal and return an idealized picture of the electro-optical properties. Alternate methods of describing the director configuration have been presented recently by Becker[2] *et al.* or Heynderickx and De Raedt.[6] A disadvantage of this approach is the high computing capacity necessary and the potential of disregarding all the subtle effects caused by imperfections and limitations of the cell itself. These limitations are avoided when experimental investigations with a test cell are made. On the other hand, a merely experimental determination of the optical slope often results in time consuming trial and error procedures when optimizing for a specific application. Clearly, an efficient and easy means for many applications is the intermediate case where a simple numerical approach is capable of estimating the optical slope for a given cell type, *e.g.* a standard test cell. The work of Schadt and Gerber[9] may provide an answer to some of the questions raised above. In their approach the optical slope is parameterized in K_{33}/K_{11} with $d{\cdot}\Delta n/\lambda$ as the independent variable. However, their formulation allows optimization in regard of these quantities only. The advantage of using the analytical approach of Raynes[7,8] for the work below is its proper consideration of K_{11}, K_{22}, K_{33}, and $\Delta\epsilon$ together, a circumstance Schadt and Gerber[9] were also aware of.

In this contribution it is shown that the calculated mid-plane tilt angle for a twisted nematic configuration correlates well with the measured optical slope in respective TN test cells. Once the correlation is known (which implicitly takes into account $d{\cdot}\Delta n$, the conditions under which the set-up is illuminated, bias tilt angles, surface coupling energies and other cell specific parameters) one is in a position to estimate the optical slope as a function of the elastic constants K_{11}, K_{22}, K_{33}, $\epsilon_{\parallel}$ and $\epsilon_{\perp}$, and the twist angle. Of course, the value of the slope computed in this way is relevant only for the configuration with which the correlation has been established. The proposed method thus *can* speed up optimization when some initial experimental data are available, it *cannot* be a substitute for a theoretical treatment being independent of any measured data.

II. NUMERICAL APPROACH

A rigorous treatment of the interdependence of the twist angle ϕ and tilt angle ϑ as a function of applied voltage was first given by Deuling.[4,5] In a more extensive approach Berreman published not only a different numerical approach to describe the static deformation pattern, but also treated the dynamic behavior of various cell types. Recently, Raynes[7] provided a simple analytical expression for the initial slope of the mid-plane tilt angle ϑ_{max}. This approach takes into account the first two terms in Deuling's[5] solution and neglects higher order contributions. In a subsequent work of Raynes[8] the addition of a chiral dopant was explicitly taken into account. The formula is valid only for voltages in the vicinity of the threshold voltage. In his formulation he can also include an added chiral dopant. He could show that for angles of up to 30° his estimates of the mid-plane tilt angle ϑ are in close agreement with Berreman's computer simulations. The bias tilt was set to zero in these cases. The work presented here relies in part on the expressions given by Raynes.[7,8]

Following the general definition of the optical slope of a liquid crystal cell, one may write

$$M = [(V(10) - V(50))/V(10)] \cdot 100\% \tag{1}$$

where V(10) and V(50) are the applied voltage yielding transmission values of 10% and 50%, respectively. It is interesting to note that this slope is normalized to V(10) (and not to a transmission difference). The reason for this is to provide a means of comparing materials with different threshold voltages in view of the multiplexability in the display. Also, small M values represent steep slopes, and vice versa.

In analogy to the definition of the optical slope, one might introduce a corresponding slope defined by the voltages necessary to orient the mid-plane director as follows:

$$P = [(V(\vartheta_1) - V(\vartheta_2))/V(\vartheta_2)] \cdot 100\%. \tag{2}$$

$V(\vartheta_1)$ and $V(\vartheta_2)$ stand for the voltages necessary to achieve mid-plane tilt angles of ϑ_1 and ϑ_2. Ideally, one would like to use tilt angles ϑ corresponding to 10% and 50% of the transmission, in analogy with the definition of the optical slope. However, there is no straight translation of the mid-plane tilt angle into an optical quantity. Therefore we make the assumption that a qualitative relation between mid-plane tilt angle and optical slope exists. It is shown below that such a relation indeed is present. Further, the proper values of the tilt angles ϑ_1 and ϑ_2 had to be determined. A choice of ϑ_2 which is too large would mean that Raynes'[7,8] analytical approach would break down. A comparison of detailed computer modelling with the analytical approach verified that this is the case for angles ϑ greater than 30°. On the other hand, a choice of ϑ_1 which is too small would give excessive weight to director configurations close to the Freedericksz transition. Numerical experiments had shown that ϑ_1 and ϑ_2 set to 9° and 18° respectively returned good results. Of course, these two values did not represent optical transmissions of 10% and 50%. As a consequence, a comparison between the "optical" and "mid-plane tilt" slope is expected to be subjected to an additional scaling factor.

By using Raynes'[7,8] approach, it is possible to obtain an expression for V(ϑ) which in turn can be substituted into equation (2):

$$P = \frac{(F(K) + \gamma) \cdot V_c/4 \cdot (\vartheta_1^2 - \vartheta_2^2)}{(F(K) + \gamma) \cdot V_c/4 \cdot \vartheta_2^2 + V_c} \tag{3}$$

The expressions $F(K) = f(K_{11}, K_{22}, K_{33}, \phi)$ and $V = f(K_{11}, K_{22}, K_{33}, \phi, \gamma)$ correspond to Raynes' formulas [4] and [3]:

$$F(K) = \frac{K_{33} - \left(\frac{\phi}{\pi}\right)^2 \left\{\frac{K_{33}^2}{K_{22}} + K_{22}(1 + 4\beta + \beta^2) + K_{33}(2\beta - 1)\right\}}{K_{11} + \left(\frac{\phi}{\pi}\right)^2 \{K_{33} - 2K_{22}(1 - \beta)\}}$$

$$V_c = \sqrt{\frac{\pi^2 K_{11} + \phi^2 \{K_{33} - 2K_{22}(1 - \beta)\}}{\epsilon_0(\epsilon_{\|} - \epsilon_{\perp})}}$$

K_{11}, K_{22}, and K_{33} are the elastic constants of the liquid crystal, and ϕ is the total twist angle, γ stands for

$$\gamma = \frac{\epsilon_{\|} - \epsilon_{\perp}}{\epsilon_{\perp}}.$$

By applying equation (3) it is possible to calculate in a simplistic way the quantity P which can be correlated with the measured optical slope M of a liquid crystal display.

III. GENERAL DISCUSSION

The quantities entering the definition of the initial slope of the Freedericksz transition are K_{11}, K_{22}, K_{33}, $\epsilon_{\|}$, $\epsilon_{\perp}$, twist angle ϕ, and (implicitly) β for the chiral additive. The quantity $\beta = (2\pi d/P\phi)$ was set to zero for this work. In commercially available liquid crystal materials the three elastic constants may vary within the ranges 7.5–15, 4.5–10, and 10–25 (in units of pN), respectively. Depending on the specific mixtures, the values for $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ are between 5–40, and 3–12, respectively. The twist angle ϕ may be any value suitable for application.

The dependence of the optical slope M (or P) on these quantities is not a simple one, since even in the adopted simplification six variables are present in the expression. However, a few basic comments can be made immediately.

As already addressed by Raynes, for any given set of parameters an optimum twist angle ϕ exists for which the optical slope becomes extremely steep. A practical consequence of this is that a given mixture may show poor results in one specific test cell while it is excellent in others having a different twist angle. This effect may largely account for reported problems of display manufacturers when establishing a rank among potentially useful liquid crystalline mixtures. The manufacturers of mixtures usually have to optimize a product not only in terms of the elastic constants and the dielectric anisotropy, but also for viscosity and clearing point, which often necessitates compromises for the other parameters. Results can be improved if the twist angle is properly adjusted.

From the above formulas it can also easily be seen that a scaling factor for all elastic constants does not effect the optical slope as defined above. This is to say that there is no difference whether the elastic constants K_{11}, K_{22}, K_{33} of the liquid crystal material are 10, 5, 10, or 20, 10, 20 pN, respectively. The hypothetical scaling factor of 2 in this example would cancel out in expression (3). However, it would not cancel in the determination of the threshold voltage V_c which is proportional to the square root of this factor. A diagram showing the dependence of the optical slope on the K ratios and the dielectric anisotropy is given below.

IV. COMPARISON WITH EXPERIMENTAL DATA

Before establishing the correlation between the measured and computed optical slope as explained in Section I a comparison of the measured and computed threshold voltages for various mixtures was necessary. This step was intended to exclude an improper value of V_c as a potential source of error. For this purpose about 70 different liquid crystalline mixtures with both elastic constants and threshold voltages determined experimentally in the R&D laboratory of E. Merck were selected. Figure 1 shows a plot of the computed threshold voltages versus the measured threshold voltages. From this diagram

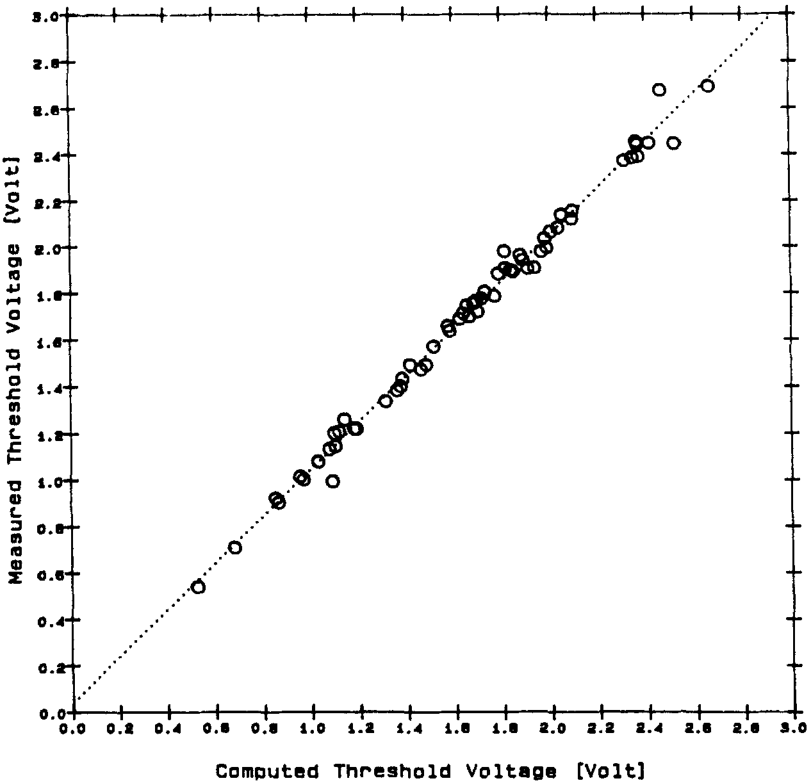

FIGURE 1 Measured threshold voltage vs. computed threshold voltage V_c for a set of liquid crystalline mixtures available from E. Merck. The measured values were obtained by evaluating the birefringence pattern in a varying electric field.

it is obvious that the threshold voltage V_c, characteristic of the Freedericksz transition, can be predicted to a high degree of accuracy.

For the subsequent comparison of computed with experimental data we used TN-cells with spacings between 5 and 10 μ, depending on the mixture parameters and whether the experiment was carried out in the first or second minimum. In contrast to V_c, *i.e.* the true initial threshold, as measured for Figure 1, a voltage reading which is often used to characterize the onset of a change in transmission is V(10). This value is of course considerably higher than V_c since the liquid crystal has undergone distinct reorientation at this point. A diagram showing V(10) as a function of V_c is given in Figure 2. It is interesting to note that there exists a linear relationship. The sets of data for the first and second minimum are well separated. For a given V_c the corresponding V(10) is consistently lower in the first minimum

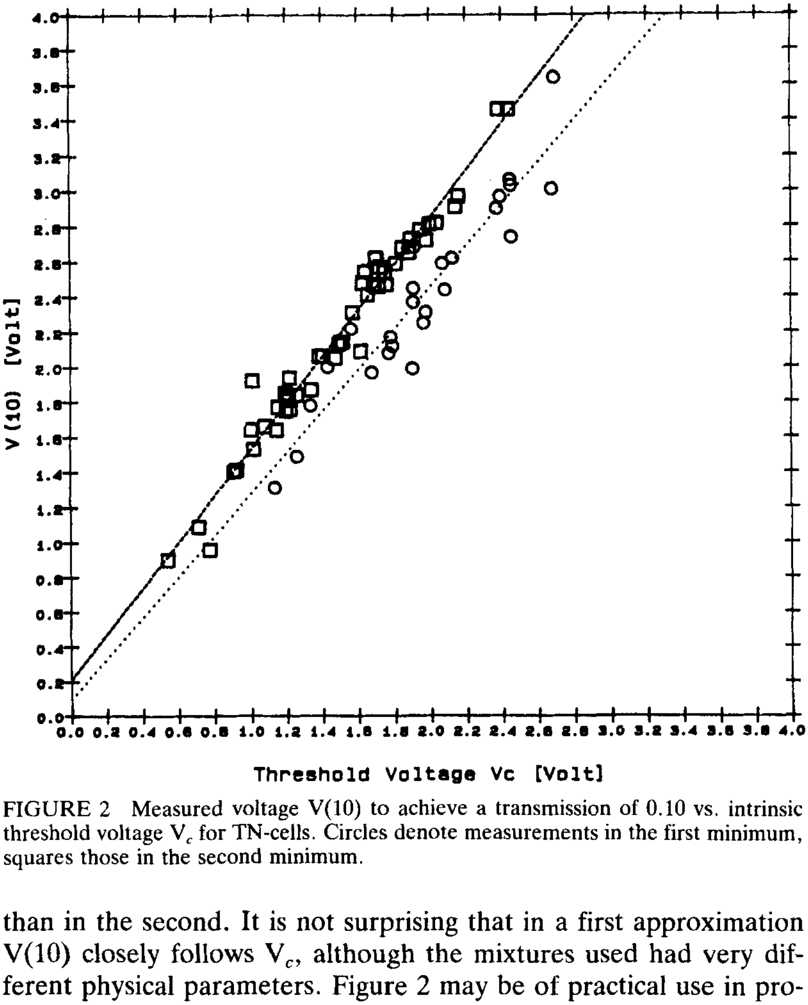

FIGURE 2 Measured voltage V(10) to achieve a transmission of 0.10 vs. intrinsic threshold voltage V_c for TN-cells. Circles denote measurements in the first minimum, squares those in the second minimum.

than in the second. It is not surprising that in a first approximation V(10) closely follows V_c, although the mixtures used had very different physical parameters. Figure 2 may be of practical use in providing a simple means to estimate V(10) for various liquid crystalline materials.

The optical slope according to (1) was measured by using standard procedures. For the evaluation given below, measurements in the first and second minimum were treated separately, due to their different characteristics.

When comparing the measured slope with the unscaled number of (3), one has to decide whether to seek a correlation of M vs. P or of $1/M$ vs $1/P$. The former relationship relies on the generally accepted convention but leads to crowding where the steep (and more reliably measurable) mixtures are located. The latter representation has the advantage of spreading the mixtures over a wider range and thus avoids cumbersome problems due to the weighting of the data. Both representations were evaluated for this contribution and are given in Figures 3 and 4. From Figure 3 one can see that $1/P$ and $1/M$ can be linked by a linear relationship. No weighting of the individual data points had been performed. The relation is somewhat less evident in Figure 4 where P vs. M is given. It is difficult to decide which one is superior, but in view of the objections mentioned above, the relationship of the inverse quantities was chosen. All subsequent discussion is thus restricted to Figure 4.

For the particular set-up used for this contribution, one can read from Figure 3

$$1/P = 3.16 \cdot 1/M - 0.14 \quad \text{(first minimum)}$$

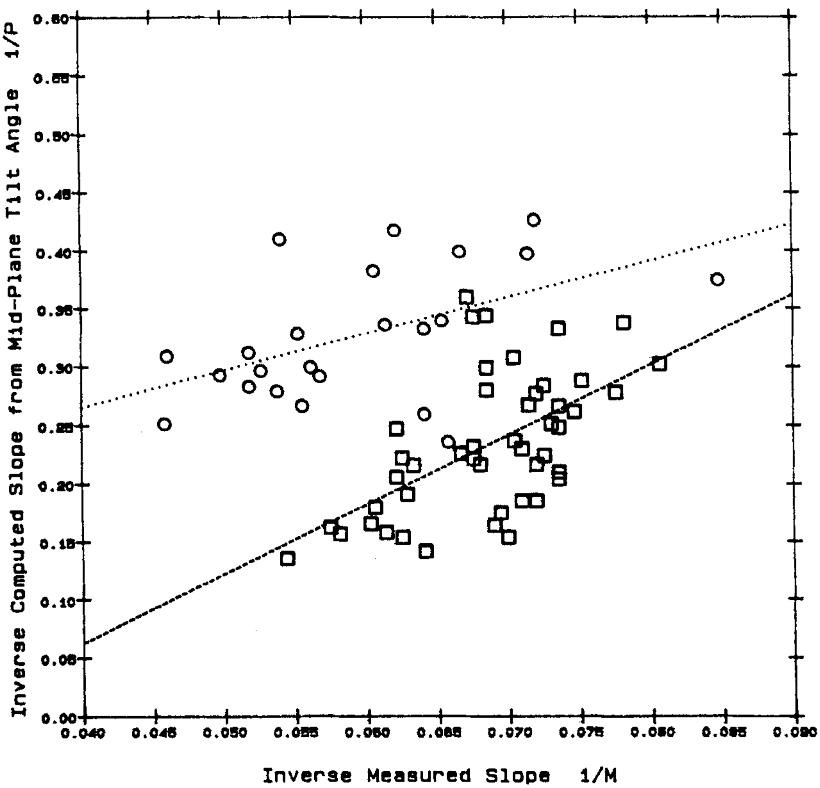

FIGURE 3 Dependence of the computed quantity $1/P$ on the measured optical slope $1/M$ for TN cells.

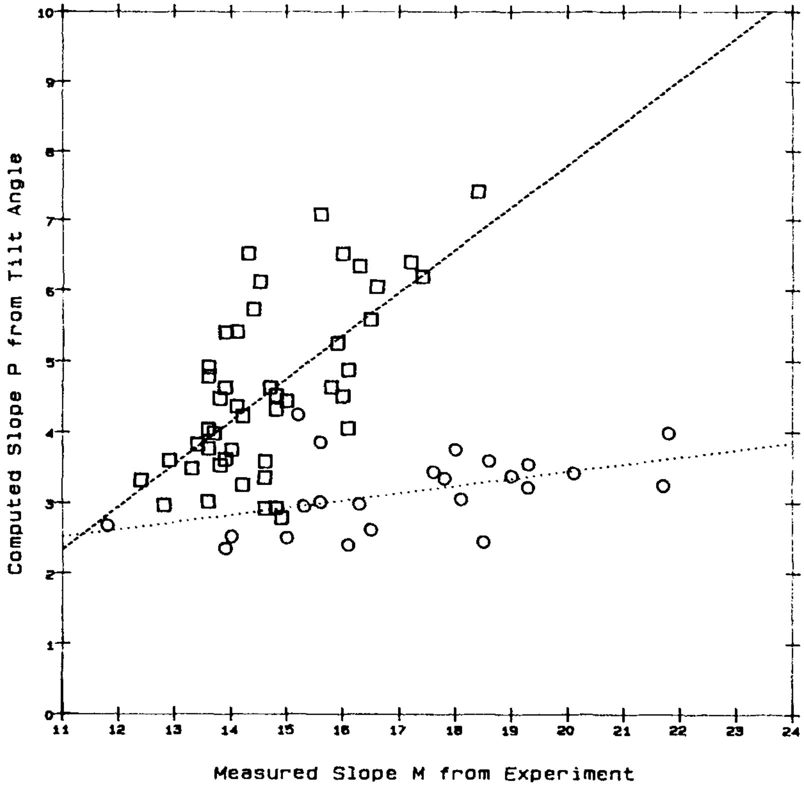

FIGURE 4 Same as Figure 1, but for M vs. P. For more details see text.

and

$$1/P = 5.98 \cdot 1/M - 0.18 \quad \text{(second minimum)}$$

It is obvious that Figure 3 is not without scatter. Although a single cell *type* had been used for the measurements presented here, *individual* cells were employed every time. These cells differed slightly in thickness. In a series of control measurements one specific liquid crystal mixture was used in a variety of individual test cells for which very exact measurements of the thickness were available. These tests show that indeed some scatter is introduced in this way. Figure 5 graphically represents the optical slope for a particular mixture (ZLI-3240) vs. $d \cdot \Delta n$ (the second minimum corresponds to 1.04 at 550 nm). Hence part of the scatter present in Figure 3 is not related to the

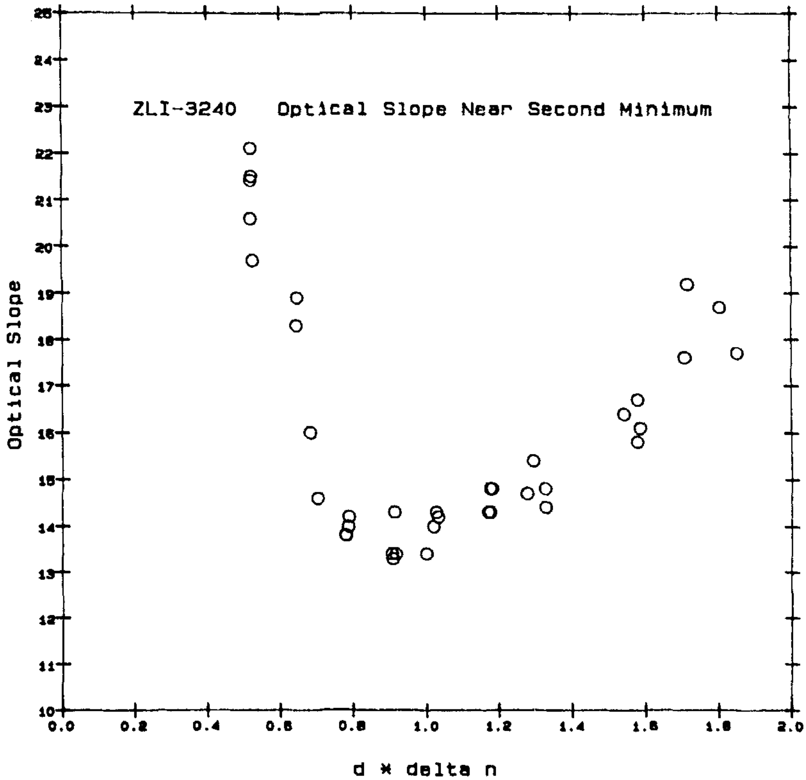

FIGURE 5 Optical slope for ZLI-3240 vs. $d \cdot \Delta n$. All other parameters were kept constant.

accuracy of the method developed here but may merely reflect the offset from the Gooch–Tarry minima.

V. CONCLUSION

In Section III it was shown that for a given experimental set-up and given test cell characteristics a linear relation of the inverse measured optical slope $1/P$ with a computed quantity $1/M$ exists. By knowing this relation and the elastical and optical properties of any other liquid crystal material it is possible to compute $1/M$, and to convert this number to an optical slope P.

This method is particularly valuable when developing a specific display and optimizing the electro-optical properties of the device. Although far from being a definitive treatment, this method is helpful when establishing a qualitative grade of various materials. As pointed out in Section II the twist angle ϕ is also an independent variable and should properly be taken into account.

Subsequently, an estimate of the dependence of the optical slope M on various physical parameters by applying expression (3) may be achieved. Since the expression used to derive (3) is based on the first two terms of the rigorous analytical formula only and since several other parameters are accounted for only by means of the correlation, the results should be considered as solely qualitative. However, the result of (3) correlates well with *e.g.* results based on Berreman's code published by Baur.[1]

In Figure 6, M is plotted versus the ratio K_{33}/K_{11} as the independent variable. The twist angle was set at 90° *i.e.* a TN cell. The ratio K_{22}/K_{11} is additionally parameterized to values of .3, .5, .7 as dotted,

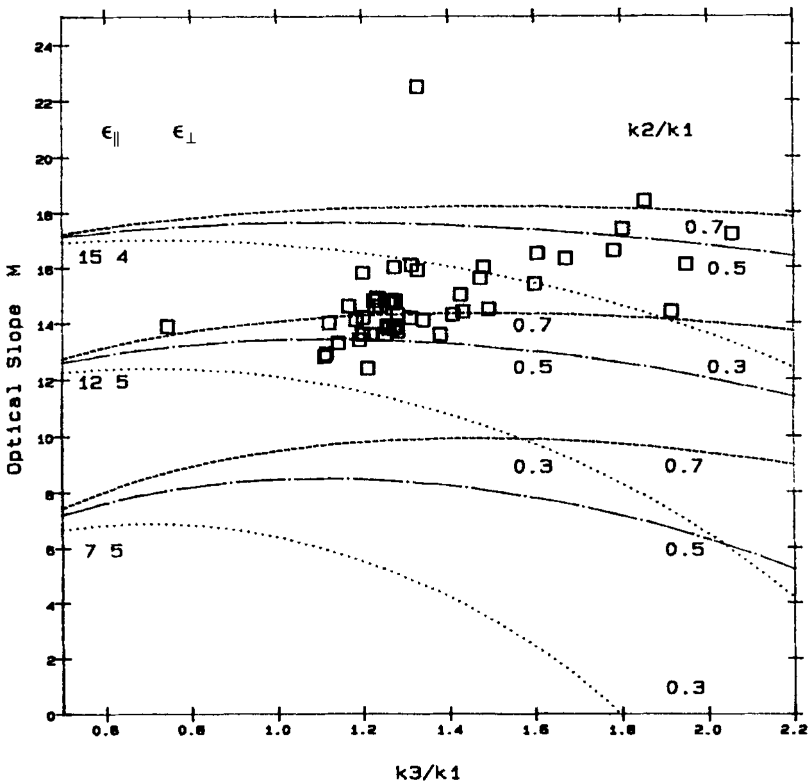

FIGURE 6 Optical slope vs. K_{33}/K_{11}. The broken lines stand for the other parameters as indicated. Squares denote measured data (second minimum).

dash-dotted, and dashed lines. There are three main groups of curves expanding from the left of the graph. Within each group the dielectric constants are fixed. $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ were for the top, middle, and bottom sets of curves chosen as 15/4, 12/5, and 7/5, respectively. Not all these values are found in the quoted combinations for commercially available mixtures, in particular regarding the range of elastic constants. More typical parameters are those of the uppermost set. The loci of the individual mixtures (measured values) are denoted by squares.

The main conclusion to be drawn from Figure 6 is that when optimizing a mixture requiring a steep optical slope the elastic constants and the dielectric anisotropy are equally important. In order to achieve good results it is not sufficient to vary solely K_{33}/K_{11}, but one also has to adjust K_{22}/K_{11}. In addition, proper consideration of $\Delta\epsilon$ is of no less importance. Given a particular value of K_{33}/K_{11}, the general trend is that for a steeper optical slope the ratio K_{22}/K_{11} should be small, and $\Delta\epsilon$ be small, too. A small dielectric anisotropy would also necessitate a high threshold and driving voltage which due to recent improvements in technology may be possible soon.

Acknowledgments

The authors are indebted to L. Pohl for stimulating discussions. The laboratory staff of FO IC PAN/P assisted in preparing the manuscript.

References

1. Baur, G., EIAJ & JSPS Symposium on Liquid Crystal Displays, Tokyo (1986).
2. Becker, M. E., Kosmowski, B. B. and Mlynski, D. A., *Proc. of the SID*, **26**, 109 (1985).
3. Berreman, D. W., *Phil. Trans. Roy. Soc.*, **A309**, 203 (1983).
4. Deuling, H. J., *Mol. Cryst. Liq. Cryst.*, **19**, 123 (1972).
5. Deuling, H. J., *Mol. Cryst. Liq. Cryst.*, **27**, 81 (1975).
6. Heynderickx, I., and De Raedt, H., preprint (1987).
7. Raynes, E. P., Tough, R. J. A., and Davies, K. A., *Mol. Cryst. Liq. Cryst.*, **56**, 63 (1979).
8. Raynes, E. P., *Mol. Cryst. Liq. Cryst. Let.*, **4** (1), 8 (1986).
9. Schadt, M., and Gerber, P. R., *Z. Naturforsch.*, **37a**, 165 (1982).