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Method to Reveal Spectral Lines with the Help of a Guest-Host LC Cell

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. A new application of the well-known LC guest-host effect is considered. Observed experimentally, the absorption edge shift controlled electrically can be exploited as a mean for spectral scanning. Physical and mathematical backgrounds of the idea imbodiment are discussed. Results of spectral measurements on the one experimental cell are shown to demonstrate the viability of the method.

Keywords: LC guest-host cell; instrumental contour; controlled dichroism; spectrum revealing

It is well-known that spectral characteristics of a guest-host LC cell can be changed under some external influence [1]. The reason is in following. The are some external influences (e.g., electric field switching) which can in reversible way reorient both LC matrix and dissolved dye molecules relatively of the transparent plane capillary wells. When an electric vector of the incident electromagnetic wave coincides in its direction with the transition dipole moment of the dye molecule (at appropriate frequency in the spectrum) one can observe a large value of the corresponding absorption coefficient [2]. Such a coincidence takes place usually when the dye molecules hold their transition dipole moment in parallel to one of the two orthogonal directions in the plane of the capillary. In the other orthogonal direction or when the dye transition dipole moment is perpendicular to the capillary wells the dye absorption coefficient is smaller. This phenomenon is named as dichroism.

We considered the case where the LC matrix molecules are aligned initially in planar way, i.e. in parallel to the capillary wells. When the LC matrix consists of molecules with positive dielectric anisotropy (rod-like ones or having a permanent dipole moment along of their long axes) an applied electric field of sufficient magnitude normally to the LC layer will turn from the planar orientation to perpendicular one when molecular long axes will align normally to the capillary wells. Together with the LC matrix, similar reorientation takes place for the dye molecules with their transition dipole moments. It is only sufficient for them to have an appropriate anisotropic shapes.

This is the way to change mutual orientation between direction of the dye transition dipole moment and invariable (when one wants) direction of electric vector of incident light wave. Since the molecular reorientation proceeds gradually the extent of the absorption will be also changed gradually. So, in the similar gradual manner, one can vary the spectral features of the cell which are indeed conditioned by this dichroic effect.

It is generally accepted that a visual (spectral) effect observed is due to that some spectral region around the maximum value of absorption coefficient increases or decreases in the extinction magnitude that leads to some changes in color (spectral) saturation but no spectral shift. Intuitively, this is clear because the extinction (absorption) coefficient is ordinarily varied in direct proportion for all the wavelengths from the spectral range considered.

In fact, it is true only for small absorbance. In practice, one never observes the absorption coefficient (absorbance) directly. The physical value observed for transparent bodies is ordinarily *the transmittance* or transmission coefficient defined as ratio of the transmitted radiation power to incident one. This physical quantity is regulated by the absorption coefficient but not in directly proportional manner. Well-known Lambert - Beer's law plays its role in this field:

$$T = \exp(-\alpha c d), \qquad (1)$$

where T is the transmittance, α - absorption coefficient, c - the concentration of the dye considered, and d - the thickness of the LC layer.

One can see from the eq.(1) that the more the absorption coefficient the less is the transmittance. Moreover, if one considers a new quantity, $(1 - T)$, it can be seen that for sufficiently small values

of absorption coefficients (when c and d are constant), decomposition in series on powers of the absorption coefficient shows the $(1- -T)$ is direct proportional to α for small magnitudes of the last. This is the reason for the incorrect view that the controlled dichroism can be a mean only for amplitude modulation but not for spectral-selective one.

Such a view is not correct for large magnitudes of the quantity αcd. Let us consider an absorption band that has in its minimum at a single wavelength only about 0.1 per cent of transmission (see FIGURE 1., curve *a*). Let this curve to correspond the situation where light-absorbing molecules interacts with the electric vector of electromagnetic wave in minimal extent. Then, after changing the orientation of anisometric and dichroic molecules, their absorption must increase. It is difficult to reveal further diminishing of transmission in the maximum of the absorption band. Visually, it remains at approximately the same level. But one can see considerable decreasing of transmission at other wavelengths inside of the absorption band (FIGURE 1., curve *b*). An initial level 0.1 per cent of transmission will be now exceeded in rather wide range. The magnitude of the effect depends on the extent of dichroism for the light-absorbing molecules.

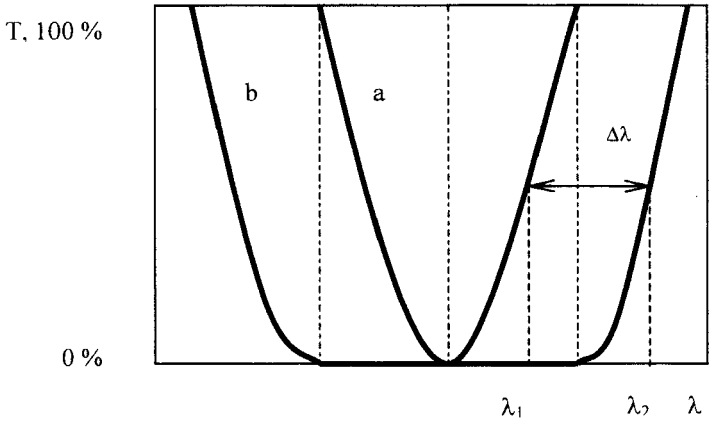
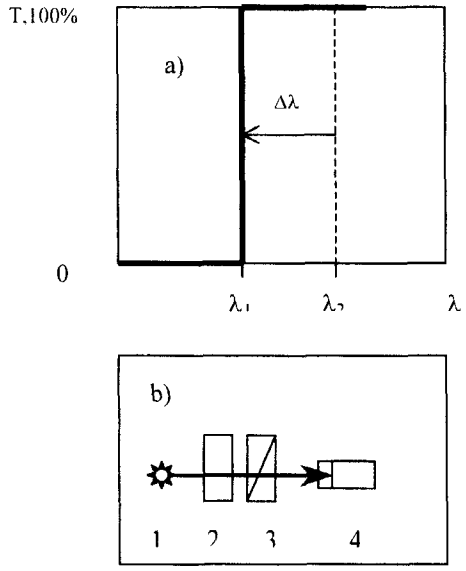


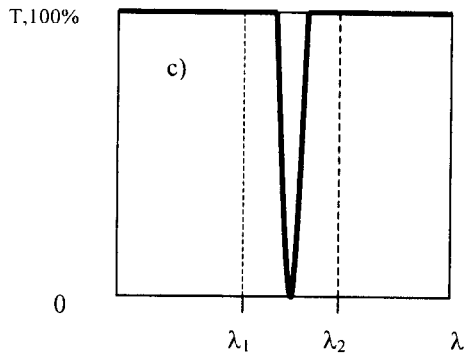
FIGURE 1. Increase of extinction within an absorption band on the transmittance scale. (a) - the orientation for minimal interaction with electric vector of light wave; (b) - the one for maximal interaction with electric vector of light wave.

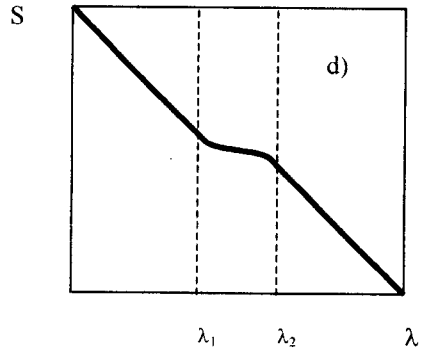
Let us consider now the spectral range between the wing of the absorption band *a* and the same of the absorption band *b* (this range is shown in FIGURE 1. by vertical dotted lines). Inside this spectral range, there is a well-determined shift of the absorption edge. Of course, gradual changing in the molecular orientation will lead to the same gradual spectral shift of the absorption band. Further, we shall consider such a spectral shift as a kind of spectral scanning.

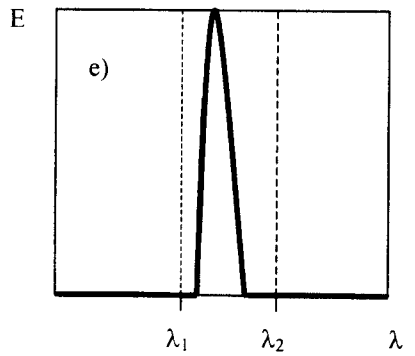
To illustrate this idea, let us begin from some simplifications. We shall now imagine the absorption edge as simple rectangular step that may move within some spectral range (FIGURE 2, a) under external influence (e.g., electric field). Let us put such an idealized LC guest-host cell between a radiation detector and a radiation source (FIGURE 2, b) emitting within the above spectral range. Now, we suppose that there is a narrow absorption peak in the continuous spectrum within this range (FIGURE 2, c). At last, let us turn on the external influence and thereby execute the scanning operation. A signal of what kind does one see on the detector?

From mathematical point of view, it is a convolution of the source spectral continuum with the absorption peak and the stepwise instrumental contour. The result of such an operation, i.e. the shape of the signal is shown in FIGURE 2, d.









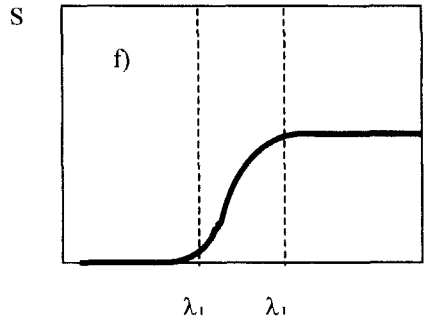


FIGURE 2. (a) An idealized absorption edge and its shift. (b) Scheme of the experiment imagined: 1 - a light source; 2 - the dichroic LC cell; 3 - a polarizer; 4 - a light detector and recording device. (c) - An example of external spectrum containing a single absorption line in the range considered. (d) - The result of convolution of the spectrum (c) with the stepwise instrumental contour. (e) - An example of external spectrum containing a single emission line. (f) - The result of convolution of the spectrum (e) with the stepwise instrumental contour.

If we imagine another case where the external spectral signal represents several (e.g., two) emission lines (FIGURE 2, e) the result of convolution will have a shape shown in FIGURE 2, f. Obviously, any external spectral signal can be represented as sum of some continuum and absorption and emission lines. The problem now occurring is to obtain a true external spectral signal from the observed result of convolution. We have several ways to solve such convolution equations (so-called deconvolution) but we omit their description for the sake of the article area. Here we note that in spite of unusual shape of the instrumental contour, the results of deconvolution coincide very well with the external spectral signal for different instrumental contour versions of that kind (rectangular step, sloping step, rounding step).

It is interesting to note that there is very simple way to reduce a true external spectral signal for the case of rectangular step. It consists in simple differentiation of an observed convolution result on wavelengths.

It was important to check experimentally this spectroscopic approach. If the spectral shift would seem to be too small it were difficult to find a good application of the effect.

The LC cell used was of standard construction with the thickness of LC layer of about 8 μm, a LC matrix was LK7 (Sevchenko Institute of Applied Physical Problems, Minsk), a dye was D2 (NIOPIK, Moscow). Firstly, the cell and an appropriate polarizer was installed in the optical path of a spectrophotometer «Specord» UV-Vis (Carl Zeiss, Jena). When the voltage (frequency 1 kHz) applied to the cell was varied from 1.2 to 8 V, the absorption edge at the 50%-transmission level was shifted from 558 to 582 nm (FIGURE 3). The slope of the absorption step observed was enough steep, so the spectral range within which the effect of the absorption edge shift yet occurred stretched from 513 to 606 nm. From these data, one can conclude that satisfactory frequency (wavelength) modulation will be possible in the range approximately from 520 to 600 nm. Such size of the range is completely suitable as most spectral features to be revealed under routine spectroscopic investigations have their spectral widths more narrow essentially. But only an experiment must be the essential criterion.

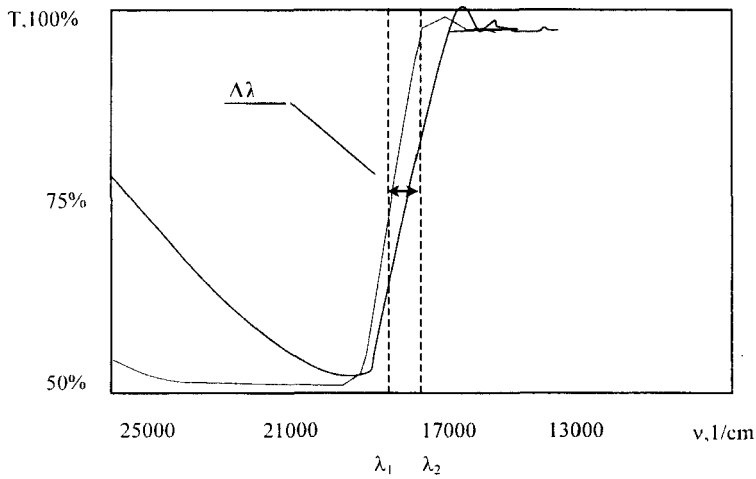


FIGURE 3. The spectral shift observed in the experiment with the LC cell containing the dye D2.

For the next step of our study, we attempted to see how the method functions under near-real conditions. Several interference filters with transmission bands within and around of the spectral range shown served as simulators of external emission lines (bands). Measurements were conducted in the same manner as above with the filter added in the optical path. The area under the transmission curve of the simulation filter was considered as a measure of convolution signal proportional to integral transmittance of the filter-cell combination. Figure 4 represents the dependences of the areas (in arbitrary units) on the voltages (in V) applied to the LC guest-host cell. The four curves correspond to the four interference filters with their transmittance peak positions at 580.5 nm (S1), 556.0 nm (S2), 532.4 nm (S3), and 507.5 nm (S4).

As it can be concluded from FIGURE 3, the so-called *scanning* is carried out in such a manner that when the voltage increases the spectral range under question is being opened gradually from large wavelengths to shorter ones. This process does be imprinted on the curves of FIGURE 4 Curve S1 corresponds to the filter of the most long wavelength (580.5 nm) where the scanning begins. So the expected increase of integral transmittance hits on the beginning of curve 1, i.e. to very small volts. Curve S2 demonstrates expected further shift of the integral transmittance increase to more high voltages (to about 2 V) because it corresponds to the ransmission peak of a shorter wavelength (556.0 nm). So one can see that simple increase or decrease of the voltage applied to the cell plays the role of a scanning influence.

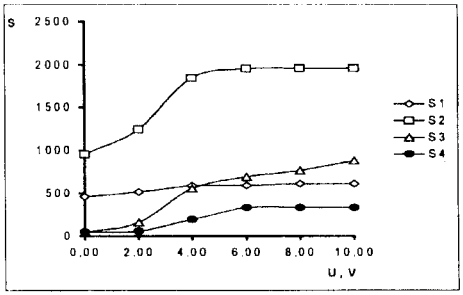


FIGURE 4. Experimental plots demonstrating the effect of convolutions for the dichroic stepwise instrumental contour and a

quasi-emission line in four different wavelength positions. Comments in the text.

Curves S3 and S4 show a further shift of the integral transmittance increase to more high voltages (about S4 and more volts) in correspondence with the wavelengths 532.4 and 507.5 nm of the filter transmission peaks. Besides, transmission peak of the last filter superposes on the boundary of the scanning spectral range where transmission of the LC cell is low for all voltages, so the result signal (integral transmittance) is less then for the other filters. Consequently, reduction of the last filter transmission peak from the integral signal (curve S4) is very questionable.

Thus in this article, we have attempted to demonstrate the possibility for development of new liquid crystal applications, namely using of the LC guest-host cells as spectral instruments of a new kind.

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