PHYSICAL PROPERTIES OF PHYTOL MEASURED BY LASER LIGHT SCATTERING

Milesa Srećković, Fedor Boreli

Faculty of Electrical Engineering, University of Belgrade, 11000 Belgrade, P.O.Box 816, Yugoslavia

Jovan Konstantinović

"Boris Kidrič" Institute of Nuclear Sciences, Laboratory of Solid State Physics and Radiation Chemistry, 11001 Belgrade P.O.Box 522, Yugoslavia

Abstract: The depolarized and polarized scattered He-Ne laser light was measured. From these measurements Rayleigh factor and depolarization factors of phytol were calculated. Based on these results the values of isothermal compressibility and molecular mass of phytol were obtained. These values are compared with corresponding results obtained with other methods.

Introduction

Phytol, $C_{20}H_{39}OH$ is unsaturated primary alcohol with one double bond. As a structural part of chlorophyll in the form of phytol group [1], it is the basic product of its decomposition. It was synthetized for the first time in 1929[2] and extracted from plants in 1943[3]. The molecular structure is not completely known[4]. The values of the refractive index[5], n_α=1.4601, n_D=1.4623, n_γ= 1.4595, molecular mass[5], from 296.54 to 296.32, and density, ρ=0.8497 g. cm^{-3}, were determined.

In this work, the measurements were performed of the scattered He-Ne laser light (λ= 632.8nm) from spectroscopically pure phytol

(Flika product) as well as from benzene solution.

The general formula for quasielastic light scattering[6] gives the intensity of the scattered light:

$$I = I_o \frac{\pi^2}{\lambda^4 r^2} V\{(\frac{\partial \varepsilon}{\partial \rho})_T^2 \overline{\Delta\rho^2} + (\frac{\partial \varepsilon}{\partial T})^2 \overline{\Delta T^2}\} v \sin^2\phi \frac{6+6\Delta u}{6-7\Delta u} \quad (1)$$

where: I - intensity of scattered light; I_o - intensity of incident light; λ - wavelength; r- distance between the detector and the scattering center; V - volume of the sample; ε - dielectric constant; T - temperature, ρ - density; v- volume element of the scatterer ; ϕ - angle between the electric vector of incident light wave and radius vector; Δ_u - depolarization factor for natural light

$\overline{\Delta\rho^2}$ and $\overline{\Delta T^2}$ are mean square fluctuations of density and temperature, respectively:

$$\Delta\rho^2 = kT \frac{\beta_T \rho^2}{v} \quad ; \quad \Delta T^2 = kT^2/\rho C_v v \quad (2)$$

where: k - Boltzmann constant, β_T - isothermal compressibility and C_v - specific heat.

If temperature dependence of dialectric constant and the influence of anisotropy are neglected, well known Einstein-Smoluchowski formula is obtained:

$$I = I_o \frac{\pi^2}{\lambda^4 r^2} V_k T \beta_T \{\rho (\frac{\partial \varepsilon}{\partial \rho})\}^2 \sin^2\phi \quad (3)$$

It is possible to consider the total intensity of scattering as formed by two components of incident light: polarized horizontally and vertically. Taking into acount, in the formula for Rayleigh scattering, the contribution of induced dipoles in the molecules of the scatterer, as well as the fact that the motion of molecules is correlated, we have for four different components of scattered light[6], for $\Theta = 90^o$:

$$I_{vv} = \frac{p}{15}(3a^2+ab^2+4ab) - \frac{q}{9}(a+2b)^2 \quad (4)$$

$$I_{hv} = \frac{1}{15} p(a-b)^2 \quad (5)$$

$$I_{vh} = \frac{1}{15} p(a-b)^2 \quad (6)$$

$$I_{hh} = \frac{1}{15} p(a-b)^2 \quad (7)$$

where: a and b are main refractions (in the case when ellipsoidal revolutions are considered).

$$p = \alpha + 1 \qquad \alpha = \int_0^\infty d\vec{r}\, g(r)h(r) \quad (8)$$

$$q = \alpha + 1 - \beta \qquad \int_0^\infty d\vec{r} g(r) = -1 \quad (9)$$

where: $g(r)$ and $h(\overset{0}{r})$ are correlation functions.

In the case of solutions, besides the fluctuations of density, fluctuation of concentration is also important.Then, it is more convenient to express the intensity of scattered light in terms of Rayleigh factors[7].

$$R_{vv}(\Theta) = Kc\bar{M}_p(P(\Theta) - 2A_2\bar{M}_pQ(\Theta)c + 4\delta) \quad (10)$$

$$R_{vh}(\Theta) = R_{hv}(\Theta) = 3\delta kc\bar{M}_p \quad (11)$$

$$R_{hh}(\Theta) = Kc\bar{M}_p|(P(\Theta) - 2A_2\bar{M}_pQ(\Theta)c + \delta)\cos^2\Theta + 3\delta| \quad (12)$$

where: $P(\Theta)$- scattering factor; A_2- second virial coefficient; δ- factor which takes into account the influence of optical anisotropy; $Q(\Theta)$ - function of intermolecular correlation; c- concentration of solute with molecular mass M_p; N_{Av}- Avogadro constant; n_o - refractive index of solvent, and

$$K = \frac{4\pi^2 n_o^2}{\lambda_o^4 N_{Av}} \left(\frac{dn}{dc}\right)^2, \quad (13)$$

where: dn/dc - increment of refractive index.

2. Experimental

The measurements were performed on photogoniodifusimeter in the Laboratory for optics, CEN Saclay, France. The apparatus consists of a He-Ne, 5mW laser, sample holder immersed in dodecane, photomultiplier, Faradey rotator, analyser, amplifier, and digital voltmeter. It is shown schematically on Fig. 1.

The cylindrical geometry was used, since it enables the measurement of angular distribution of all four components of scattered light from 0-165^{o}. Sample holder provided the place for two cells immersed in dodecane, with the possibility of continuous comparison of the measured intensity with standard, eliminating thus the parasite effects. The laser beam enters the dodecane before being scattered by the sample and then after scattering passes through dodecane again and falls on the detector. Before each filling of the cell, either with phytol or with phytol solution in benzene, the samples were filtrated using Gelman-Metricell filters.

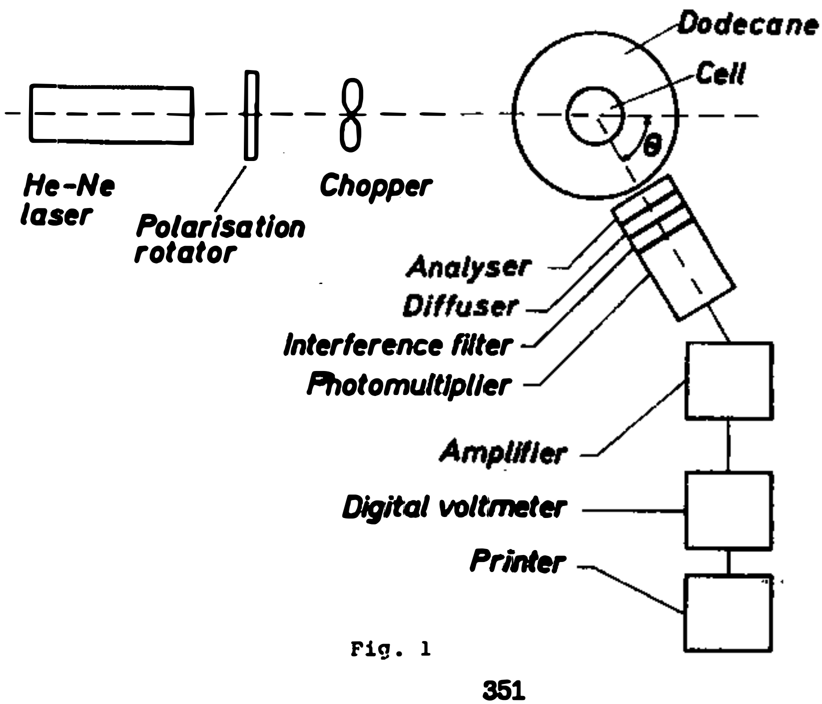

Fig. 1

3. Results and discussion

The values of the components of scattered light were measured at different angles from 30^o to 150^o (in 15^o steps).After corresponding corrections, the mean values for all four components, normalized to 90^o were obtained.

$\bar{I}_{vv} = 0.6925$

$\bar{I}_{vh} = 0.08675$

$\bar{I}_{hv} = 0.0948$

$\bar{I}_{hh} = 0.082$

From absolute measurement of the light scattered on benzene and cyclohexane[9] and measured values for I_{vv} and I_{vh}, the value of the Rayleigh factor, $R= 4.5 \cdot 10^{-6} cm^{-1}$, was obtained. From the same data, the values of depolarization factors $\Delta_u=0.223$ and $\Delta_v=0.125$, were calculated.

In order to avoid numerous corrections during the absolute measurements of the intensity of scattered light ($\theta = 90^o$), equation (1) is presented in the form:

$$I = A \cdot \left(\frac{\partial \varepsilon}{\partial \rho}\right)^2_T \Delta \bar{\rho}^2 \cdot \frac{6+6\Delta_u}{6-7\Delta_u}, \qquad (14)$$

where A is the normalization factor.

The value of normalization factor A has been determined from light scattering measurements on CCl_4 and known values for its compressibility[5]. Using the value of this normalization factor A, the compressibility of phytol was obtained from analog measurements: $\beta_T = 7.86 \cdot 10^{-10}\ m^2/N$

Taking into account the relation between the density and refractive index, the corrected values of compressibility are given in Table I, for different approximations.

It can be seen from the data given in Table I that different approximation for the values consistent within 2%.

Table I

	Lorentz-Lorenz	Eykman	ref.[6] (Vuks)
s_T (m^2/N)	$7.86\cdot10^{-10}$	$7.90\cdot10^{-10}$	$7.91\cdot10^{-10}$

The values of polarized and depolarized components of the scattered light, for scattering angle of 90° and for different concentration of phytol in benzene are given in Table II.

Table II

Concentration (g/cm^3)	I_{vv} (rel.units)	I_{vh} (rel.units)
0.04542	0.9102	0.184965
0.059567	0.969	0.186617
0.084436	0.9488	0.188312
0.1352622	0.948744	0.19089

From the dependence of I=I(c), given in Table II and the values of n=n(c)[10], the molecular mass of phytol, M=284 amu, was calculated.

Taking into account that the molecule of phytol is too small for the determination of molecular mass using the method of light scattering the obtained value is in a good agreement with the published value M= 296.54[5].

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