ALGORITHM OF DETERMINING CONDITIONS FOR NON-CATOPTRICAL ABSORPTION OF ELECTROMAGNETIC RADIATION IN POLAR LIQUID STRATA

R.M. KASIMOV, I.U. IBADZADEH, V.V. BOGATOV
Institut of Chemical problem,
Az-1143, H. Javid av., 29

The algorithm of determining conditions of non-catoptrical absorption of electromagnetic radiation in a polar liquid strata is proposed according to measurement of their static and dynamic dielectric properties.

Lately, a method of chronological radio spectroscopy based on electric pulse sounding of the substance strata with subsequent Fourier-transformation of the reflected signal [1, p.25] finds its application for express-measurement of dielectric properties of the substance in a wide frequency interval. Application of the given technique appears to be justified when thickness of the reflecting substance strata is sufficient for full dissipation of the radiation penetrating into the strata. Failure to take this into consideration may result in reception of unreliable data, especially in the course of researching weakly absorbing materials or in case of application, due to technical reasons, of measuring cells of a limited size.

At the same time, the given method may be utilized in the tasks of identifying polar liquids provided that Fourier-transformation of the total reflected signal has been conducted, i.e. with the account of finiteness of the thickness of the substance strata located in the metal measuring cell [2, p.106]. In this case, the dependence of the amplitude of reflected signal received as a result of Fourier-transformation on frequency of the incident radiation and thickness of substance strata will represent surface in the three-dimensional space, possessing a set of zero minima specific to every substance realized at a certain selective values of frequency and thickness. Existence of such a peculiar spectrum of selective strata frequency and thickness values renders an opportunity of identifying a researched substance, by comparison of its spectrum with the spectra of known substances. For realization of such an opportunity one must possess a databank of selective values of substance strata thickness and radiation frequency. They may be obtained either experimentally with application of the specified method of pulse sounding pure reference liquids, or by calculations, using literary data on their static and dynamic properties. We shall take advantage of the latter.

As has been established in the work [3, p.490], full or non-catoptric absorption of electromagnetic radiation in a flat strata of a dielectric put on a metal substrate, arises at a point of one of the wave reflection factor module dependence minima ρ from thickness l covering substance strata where the size of this minimum reaches its zero value. Conditions of existence for such function zero minimum $\rho(l)$ correspond with such selective values of dielectric permeability ε' and dielectric losses ε'' of the covering substance, which are functionally connected among themselves by the following equation:

$$\pi(2N-1)-\varphi=\frac{1}{y}ln\left(\frac{1}{r}\right), \qquad (1)$$

where $r=\sqrt{\frac{(1-n)^2+(ny)^2}{(1+n)^2+(ny)^2}}$, $\varphi=arctg\frac{2ny}{1-n^2(1+y^2)}$ - accordingly is the module and phase of wave reflection factor from the border of air-coating section; N - number of zero minimum.

Included in the equation factor of wave refraction n and factor of dielectric loss y are related with its ε' and ε'' known ratios:

$$\varepsilon'=n^2(1-y^2);\ \ \varepsilon''=2n^2y, \qquad (2)$$

At the set length of a wave λ of the incident radiation necessary to meet the conditions of its full absorption, selective thickness l covering strata is determined by expression:

$$l=\frac{\lambda}{n}\left(\frac{2N-1}{4}-\frac{\varphi}{4\pi}\right), \qquad (3)$$

One of the parameters determining existence of full radiation absorption in a substance strata, is an interval of wavelength modulation $\Delta\lambda$ or thickness Δl of the substance strata, within the limits of which the size of the reflected signal does not exceed a set in advance boundary value ρ_b. According to the research findings [4, p.737], this parameter is determined from the following equation:

$$\frac{\Delta\lambda}{\rho_b\lambda_0}=\frac{\Delta l}{\rho_b l_0}=\frac{sh(4\pi x_0y_0)}{\pi x_0}, \qquad (4)$$

where index 0 corresponds with the selective values x, y, λ and l.

For finding selective values l_0, λ_0 , as well as ε', ε'', n and y for a specific substance, one must have the knowledge of frequency dependences ε' and ε''. It is known, that in the field of its dispersion the polar liquid behavior ε' and ε'' with frequency is described by the generalized equation:

$$\varepsilon=\varepsilon'-i\varepsilon''=\varepsilon_\infty+\frac{\varepsilon_0-\varepsilon_\infty}{\left[1+(i\omega\tau)^{1-\alpha}\right]^\beta}, \qquad (5)$$

where ε_0 ,ε_∞ - is a static and high-frequency dielectric permeability; τ - time of relaxation; ω - circular frequency; α, β - empirical parameters, determining the corresponding type of dispersion. Provided that $\alpha = 0$ and $\beta = 1$ equation (5) will be transformed into the known Debye equation [1, p.25].

In certain cases the best approximation to experimental data is achieved if the substance wave dispersion is represented as a superposition of two or three dispersions of Debye type:

$$\varepsilon = \varepsilon' - i\varepsilon'' = \varepsilon_\infty + \sum_{j=1}^{3} C_j \frac{\varepsilon_0 - \varepsilon_\infty}{1 + i\omega\tau_j} \ , \qquad (6)$$

where j , C_j – is a number of dispersive area and its brought contribution.

From the joint solution of equations (1) - (6) may be found dependences between the required selective values l_0, λ_0 of the polar substance and its static and dynamic dielectric characteristics ε_0 ,ε_∞ , τ, α , β , C_j .

The developed algorithm of the initial system solution for equations (1) - (6) includes initial procedure of entering into the computer operational memory of values of static and dynamic dielectric characteristics ε_0 ,ε_∞ ,τ , α , β , j and C_j, of the chosen polar liquid, and the serial number N of the function zero minimum $\rho(l)$. Since according to the work [3, p.492] data, the spectrum of selective values of wavelength and thickness of the coating layer has low-frequency and high-frequency branches, calculation of the required parameters was carried out in two stages with subsequent calculation result conclusion for each of the calculation stages. At both stages of calculation was carried out search of values n and y, being the roots of equations (1) and (5), (6). Thus the size $z=ln(\omega\tau)$ was used as the varied parameter, modulating within limits ($-\infty$, 0) or (0, ∞) accordingly in calculations λ_0 and l_0 of the low-frequency and high-frequency branches of their spectrum. As a criterion of the calculation program stop were accepted achievements within the limits of set accuracy of the equality of values y, calculated according to equations (1) and (5),(6).

According to the developed solution algorithm, near the preset value z from equation (5) or (6) were corresponding values ε' and ε'' ; thus, in case of application of equation (5) were used expressions following there from:

$$\varepsilon' = \varepsilon_0 + (\varepsilon_0 - \varepsilon_\infty) B \cos\varphi\beta \ ; \ \ \varepsilon'' = (\varepsilon_0 - \varepsilon_\infty) B \sin\varphi\beta \, , \qquad (7)$$

where $\varphi = arctg \dfrac{A \sin 0{,}5\pi(1-\alpha)}{1 + A\cos 0{,}5\pi(1-\alpha)}$;

$$A = \exp[z(1-\alpha)] \ ;$$

$$B = \left[\frac{\cos\varphi}{1 + A\cos 0{,}5\pi(1-\alpha)} \right]^{\beta} . \qquad (8)$$

Obtained values ε' and ε'' were then used for calculations of n_D and y_D on equations (2) transformed according to these parameters:

$$y_D = \frac{\sqrt{\varepsilon'^2 + \varepsilon''^2} - \varepsilon'}{\varepsilon''} \ ; \quad n_D = \sqrt{\frac{\varepsilon''}{2y}} \ . \qquad (9)$$

Thus found values n_D and y_D have been used as initial estimates in the course of iterative procedural calculation of y_K as per equation (1), but transformed to the following type:

$$y = \frac{\ln r}{\varphi - \pi(2N-1)} \ . \qquad (10)$$

The obtained according to (10) during iteration resulting y_K value was compared with y_D and, in case of their non-conformity, a repeated calculation of both values was carried out, but with the change of Δz of the variable z. Modification of the z value is carried on until the following condition is met:

$$|y_K - y_D| \le \delta \ , \qquad (11)$$

where δ– is a set in advance accuracy of y value definition.

Thus obtained values of n_D and y_K therefore, corresponded to their selective values, i.e. to such figures under which is met the condition of full incident radiation absorption in the layer of the chosen polar liquid. With these values n_D, y_K and the set values of static and dynamic dielectric parameters of liquid, the required selective incident radiation wavelength λ_0 was determined on the equations (5) or (6), and later, by means of equations (3) and (4) accordingly, selective thickness l_0 of the liquid strata and within the limits of wavelength intervals and strata thickness, the value of the reflected signal does not exceed the boundary value ρ_b

For solution of the set task it has been resolved to take advantage of the modern MS Visual Basic 6.0 software developing environment. Results of calculations are automatically collected and displayed by such programs as MS Word or Excel, and also may be directly entered into MS Access database.

Search of the required selective values of y_K and n_D for each N is completed in case of meeting condition (10) | y_K - y_D|<< δ. On found thus values of y_K and n_D a calculation of the required selective values the wavelength λ_0 is carried out, as well as strata thickness l_0, dielectric penetrability $\varepsilon'$and dielectric losses ε''. Since the frequency spectrum of radiation and substance strata thickness contains low-frequency and high-frequency branches, calculations were carried out in two stages, described by a choice of the h iteration range.

The discovered required values are displayed in text field windows to which attributes the found values are given. The results of calculations are entered in MS Word or Excel file in direct access (Append) mode at operator's discretion.

Results of such solution of the equations (1)-(4) are illustrated by Table 1 depicting data of calculation λ_0, l_0 of some polar liquids possessing wave dispersion with known values of relaxation time τ, static ε_0 and high frequency ε_∞ dielectric penetrability, as well as empirical parameters α, β. Consequently, this implies that any polar liquid, possessing wave dispersion within certain frequency range, has therein a strictly determined and inherent in the given liquid spectrum of selective values of the substance wavelength and strata thickness, corresponding with the conditions of full radiation absorption within the substance. The spectrum consists of a low-frequency and high-frequency branches, distinguished by the nature of selective wavelength change with increase of selective substance strata thickness. Thus, with increase of N figure, and consequently, the selective thickness l_0 of the substance strata as well, a spike λ_0 occurs for a low-frequency branch of the spectrum and its reduction for high-frequency branch appropriately. Distinctive feature of selective full absorption of electromagnetic radiation is a probability of spectrum degeneration in view of smallness of value ε_0 , in particular in case of substances with weak polarity, such as an anisole, chloroform, etc. Spectrum decline is manifested in absence of lines therein, corresponding to small N values.

Table 1

Selective values of wavelength λ_0 and thickness l_0 of some polar liquids' coating strata for low-frequency and high-frequency branches of non-catoptric wave absorption spectrum. ε_0, ε_∞, τ - implies both static and high-frequency dielectric permeability and liquids' relaxation times.

№	Liquid	N	Low frequency spectrum branch			High frequency spectrum branch		
			λ_0 cm	l_0 cm	$\frac{\Delta\lambda}{\rho_b\lambda}$	λ_0 mm	l_0 mm	$\frac{\Delta\lambda}{\rho_b\lambda}$
1	Acetone	1	1,943	0,111	0,579	0,470	0,092	1,726
	ε_0=21,2	2	6,144	1,008	0,193	0,195	0,108	0,996
	ε_∞=1,9	3	10,36	2,822	0,116	0,123	0,112	0,687
	$\tau=3{,}23\cdot10^{-12}$ s	4	14,60	5,560	0,083	0,089	0,114	0,517
	α=0,02; β=1	5	18,86	9,226	0,065	0,070	0,114	0,413
2	Acetonitrile	1	3,522	0,154	0,444	0,244	0,042	1,584
	ε_0=36,23	2	13,62	1,716	0,146	0,080	0,041	0,896
	ε_∞=2	3	24,89	5,201	0,087	0,046	0,040	0,816
	$\tau=3{,}8\cdot10^{-12}$ s	4	37,00	10,80	0,062	0,031	0,038	0,465
	α=0,14, β=1	5	49,55	18,58	0,048	0,023	0,037	0,372
3	Acetophenone	1	3,079	0,211	0,689	1,470	0,191	1,247
	ε_0=18,66	2	21,31	3,822	0,213	0,255	0,114	0,699
	ε_∞=2,45	3	45,87	13,51	0,126	0,121	0,093	0,473
	$\tau=7{,}4\cdot10^{-12}$ s	4	74,73	30,63	0,090	0,076	0,083	0,355
	α= 0,28, β=1	5	107,0	56,25	0,069	0,053	0,075	0,283
4	1-Butanthiol	1	---	---	---	---	---	---
	ε_0=5,21	2	2,933	1,018	0,475	2,910	1,360	0,743
	ε_∞=2,085	3	5,475	3,053	0,278	1,220	0,994	0,533
	$\tau=9{,}4\cdot10^{-12}$ s	4	7,860	6,081	0,198	0,713	0,828	0,411
	α=0, β=0,65	5	10,22	10,15	0,154	0,481	0,724	0,332
5	Pentandiol	1	---	---	---	---	---	---
	ε_0=4,85	2	---	---	---	---	---	---
	ε_∞=2,094	3	9,352	5,442	0,296	2,810	2,190	0,490
	$\tau=24{,}3\cdot10^{-12}$ s	4	13,86	11,15	0,209	1,360	1,536	0,384
	α=0, β=0,5	5	18,19	18,72	0,162	0,813	1,182	0,314
6	Diethyl ether	1	---	---	---	---	---	---
	ε_0=4,36	2	1,085	0,411	0,539	1,330	0,721	0,952
	ε_∞=1,845	3	1,935	1,180	0,318	0,793	0,726	0,688
	$\tau=2{,}44\cdot10^{-12}$ s	4	2,745	2,323	0,226	0,561	0,732	0,529
	α=0, β=1	5	3,553	3,851	0,176	0,439	0,726	0,427
7	Diethyl phthalate	1	---	---	---	---	---	---
	ε_0=7,86, C_1=0,829	2	87,94	24,15	0,350	41,970	17,215	0,605
	ε_{x1}=3,31 ε_{x2}= 2,37,	3	151,0	67,96	0,209	2,883	2,234	0,482
	$\tau=133\cdot10^{-12}$ s,	4	213,0	133,6	0,149	1,725	1,926	0,376
	$\tau=2{,}5\cdot10^{-12}$ s,	5	221,3	221,2	0,093	1,276	1,844	0,302

Since every substance possesses an individual spectrum λ_0, l_0, its experimental identification and comparison with initially found spectra of known substances makes possible identification with their means of unknown researched substances.

[1] *Y.Yu. Akhadov*. Dielectric parameters of pure liquids. Moscow. Publ. H. MAI.1999, p. 812.

[2] *R.M. Kasimov, Ch.O. Kajar, E.R. Kasimov, S.R. Gasanov*. Azerb. Rep. Patent. 2005.

[3] *R.M. Kasimov*. Magazine of engineering and physics, 1994, v. 67, № 5-6, p.489.

R.M. Qasımov, İ.U. İbadzadə, V.V. Boqatov

POLYAR MAYE TƏBƏQƏSİNDƏ ELEKTROMAQNİT ŞÜALANMANIN TAM UDULMASI ŞƏRTLƏRİNİ MÜƏYYƏNLƏŞDİRƏN ALQORİTM

Statik və dinamik xassələrin ölçülməsi əsasında polyar maye təbəqəsində elektromaqnit şüalanmanın tam udulması şərtlərini müəyyənləşdirən alqoritm təklif olunmuşdur.

Р.М. Касимов, И.У. Ибадзаде, В.В. Богатов

АЛГОРИТМ ОПРЕДЕЛЕНИЯ УСЛОВИЙ БЕЗОТРАЖАТЕЛЬНОГО ПОГЛОЩЕНИЯ ЭЛЕКТРОМАГНИТНОГО ИЗЛУЧЕНИЯ В СЛОЕ ПОЛЯРНОЙ ЖИДКОСТИ

Предложен алгоритм определения условий безотражательного поглощения электромагнитного излучения в слое полярной жидкости по данным измерения их статических и динамических диэлектрических свойств.

Received: 16.03.07