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Electron Phenomenological Spectroscopy and Its Application in Investigating Complex Substances in Chemistry, Nanotechnology and Medicine

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Abstract: The original electron phenomenology spectroscopy methods of determining physicochemical properties and characteristics of electronic structure of multicomponent and complex molecular systems have been generalized. In basic of the considered methods physicochemical properties have been estimated according to phenomelogical quantum characteristics of all electron states of the investigated system such as: integral oscillator strength in ultra violet (UV), visible and neer infrared radiation (IR) electron spectrum region and color characteristics. Physicochemical properties definition is based on the law of the connection among this properties and quantum continuum characteristics of different systems. The exampeles of using this metods in chemistry, chemical engineering, nanophysics and medicine are shown.

Key words: Electronic phenomenological spectroscopy, quantum continuum of electron states, complex organic systems, physicochemical properties, reactionary ability, color characteristics.

1. Introduction

Despite the progress in the experimental and quantum methods, there are significant discrepancies in some cases between the predicted values and the experimental results of the electron structure determination of complex materials and compounds. Therefore, it is necessary to create new methods of physicochemical properties (PCPs) and electron structures estimation, for example, the ionization potentials (IP), the electron affinities (EA), the work functions and some other properties. The knowledge of PCPs and the electron structure of complex systems and materials has fundamental importance for solving problems in many fields of science and technology, for example, physics of solid state, chemistry, electronics, and nanotechnology. The determination of the electronic structure of molecules is a significant problem of molecular electronics and materials science. Main methods, which were proved in our previous works, will be considered in the review.

Conventional spectroscopic methods are difficult in applying for the research of multicomponent natural and biologic systems, which have a great number of components, for example: biogeochemical systems, oils, polymer mixtures, oligomers, high molecular products of polymer destruction and fuel, hydrocarbon fractions and components of human blood. The spectra of such systems in UV, visible and near IR regions have indiscrete, continuous character (Figs. 2 and 6). Such spectra contain low count of spectral bands. For such systems lack of information concerning the structure and composition of components is typical. The aim of this review is to

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represent new spectroscopic method for investigating complex and multicomponent molecular systems, electron phenomenological spectroscopy (EPS). Practical application of EPS in different areas of science and engineering will be also shown.

2. Bases of Electron Phenomenological Spectroscopy

In Refs. [1-4], the method of EPS has been discovered by Michail Dolomatov. During last years, this direction was developed by the group of Dolomatov. There are the following approaches and physical phenomena in the basis of EPS:

Unlike conventional methods, the EPS studied substances as a comprehensive quantum continuum without separating the spectrum of the substance into characteristic spectral bands on certain frequencies or wavelengths of individual functional groups or components.

New physicals phenomena appear in consideration of the integral systems which absorb radiation. For example, EPS is based on the regularities of the correlation of PCPs and integral spectral characteristics for UV or (and) visible regions of the electron spectrum. Integral spectral characteristic can be any physical value of general absorption or emission of electromagnetic radiation, such as integral oscillator strength (IOS):

$$\theta = \int_{\delta}\int_{\xi} f(\xi) d\xi d\delta \qquad (1)$$

where θ is a reflection of quantum continuum as the sum of different states of electron, for example all vibration states and electron states of transition among different levels; $f(\xi)$ is spectral function of absorption or emission of radiation; δ is a range of wavelengths or frequencies.

Therefore it follows that there is regularity between absorption coefficients and PCPs of the substance. The values of PCPs of the substance are proportional to UV and/or visible quantity of absorption radiation so-called law "spectrum-properties" [4].

Color is also an integral characteristic of a visible spectrum. Therefore, the consequence of this is so-called law "color-properties" [5].

Thus, such an unusual aspect of electron spectroscopy has been named the electron phenomenological spectroscopy because integral characteristics of the system are studied. Qualitatively new laws appear on the integral level.

In 1988-1995, as a result of generalizing the results on electron spectra of multicomponent and individual substances, it was ascertained by Dolomatov and Mukaeva [6-8], that IOS in UV, VIS and near IR areas is connected with PCPs of the substances by semiempirical dependences:

$$Z = \gamma_0 + \gamma_1 \cdot \theta + \gamma_2 \cdot \theta^2 + \gamma_3 \cdot \theta^2 \qquad (2)$$

where Z, the equilibrium physicochemical property of the radiation absorbing system, in the dimension of property; θ properties of quantum continuum including integral oscillator strength or color properties; $\gamma_0, \gamma_1, \gamma_2, \gamma_3$, coefficients which depend on the substance used and the method of measurement.

Experiments have shown that application of the logarithmic IOS function give more enhanced data:

$$\theta_{\lg} = \int_{\lambda_1}^{\lambda_2} Lg(\varepsilon(\lambda)) d\lambda \qquad (3)$$

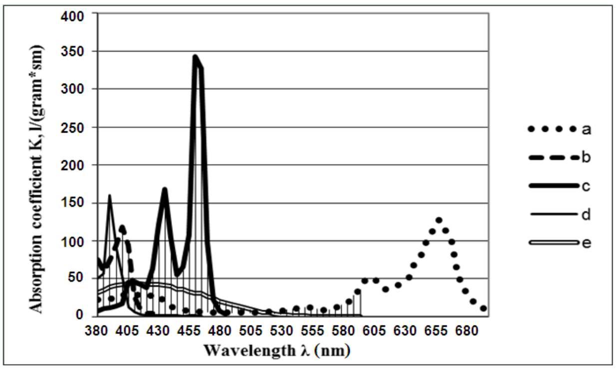


Fig. 1. Absorption spectra of the polycyclic aromatic compounds.

(a) bisantene benzene solution; (b) 1, 12-2, 3-8, 9-threebenzperylene benzene solution; (c) 1, 2-7, 8-dibenzanthanthrene benzene solution; (d) 1, 2-3, 4-9, 10-threebenzperylene ethanol solution; (e) 2-tiapyranthion ethanol solution.

Table 1 Coefficients of the Eq. (2) for noble gases.

PCP	Wavelength range λ_1-λ_2 in Eq. (3) (nm)	Coefficients of Eq. (2)			
		γ_0	γ_1	γ_2	γ_3
IP, eV	180-930	38.14	-0.02	5.41×10^{-6}	-
EA, eV	180-930	-2.77×10^{-2}	2.78×10^{-4}	3.07×10^{-8}	-

Table 2 Coefficients of the Eqs. (2) and (3) for organic compounds.

Physicochemical property	Organic compound	Wavelength range λ_1-λ_2 in Eq. (3) (nm)	Coefficients of Eq. (2)			
			γ_0	γ_1	γ_2	γ_3
Density d_c (kg/m^3)	3	200-290	273.60	1.35	1.19×10^{-2}	2.99×10^{-5}
Melting temperature T_{mel} (K)	1	200-290	239.98	-0.39	-5.74×10^{-3}	2.40×10^{-6}
IP (eV)	1, 2, 3	200-700	9.59	-4.00×10^{-3}	1.80×10^{-6}	-4.20×10^{-10}
	1	200-700	10.49	-3.40×10^{-2}	0.20×10^{-3}	2.70×10^{-7}
	2	200-700	9.05	1.70×10^{-2}	-1.60×10^{-4}	0.30×10^{-6}
	3	200-700	10.11	-7.09×10^{-3}	6.10×10^{-6}	-2.10×10^{-9}
EA (eV)	3	200-700	-0.40	2.14×10^{-3}	-5.25×10^{-7}	
		200-700	0.81	-1.91×10	3.55×10^{-6}	-1.24×10^{-9}

1 unsaturated hydrocarbon; 2 replaced molecules of benzene series; 3 polycyclic aromatic hydrocarbons.

where $\theta_{\lg}$ is the integral logarithmic index of absorption (logarithmic IOS), nm; $\varepsilon(\lambda)$ is the molar extinction coefficient, l·mole^{-1}·cm^{-1}; λ_1, λ_2 are borders of the spectrum in UV and (or) visible region, nm.

Results of the determining PCPs of noble gases and some organic molecules by Eqs. (2) and (3) are shown in Tables 1 and 2 [6-8].

Experiments have shown that in many cases quasilinear approximation is enough in the amount of the first term of Eq. (2):

$$Z = \gamma_0 + \gamma_1 \cdot \theta_{\lg} \quad (4)$$

In many processes, it is necessary to take express control of the PCPs. Therefor dynamic form of Eq. (4) has been investigated in the author's very last investigation of more than 200 of multicomponent hydrocarbon systems (Fig. 2):

$$\Delta Z = \gamma \cdot \Delta\theta_k \quad (5)$$

$$\theta_k = \int_{\lambda_1}^{\lambda_2} k(\lambda)\, d\lambda \quad (6)$$

where ΔZ is the change of the physicochemical property, $\Delta\theta_k$ is the change of IOS, × 10^{-10} m^{-3}·g^{-1}; γ is coefficient which depends on the physicochemical property, (property) × 10^{10} g·m^3; $k(\lambda)$ is an absorption coefficient on wavelength λ, l·g^{-1}·cm^{-1}; λ_1, λ_2 are borders of the spectrum in UV and (or) visible region, nm.

Results of the determining PCPs of hydrocarbon systems using integral characteristics of the absorption spectra (Fig. 2) by Eqs. (5) and (6) are shown in Table 3.

Results of analyzing 222 absorption spectra of the solutions of multicomponent hydrocarbon systems using Eq. (5) is shown in Fig. 3.

The research of the correlation among property and spectral characteristics have been carried out according to the following scheme:

Registration of absorption spectra of solutions of substances in UV and visible regions;

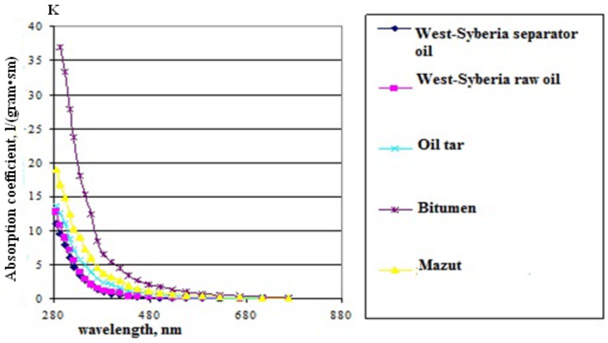
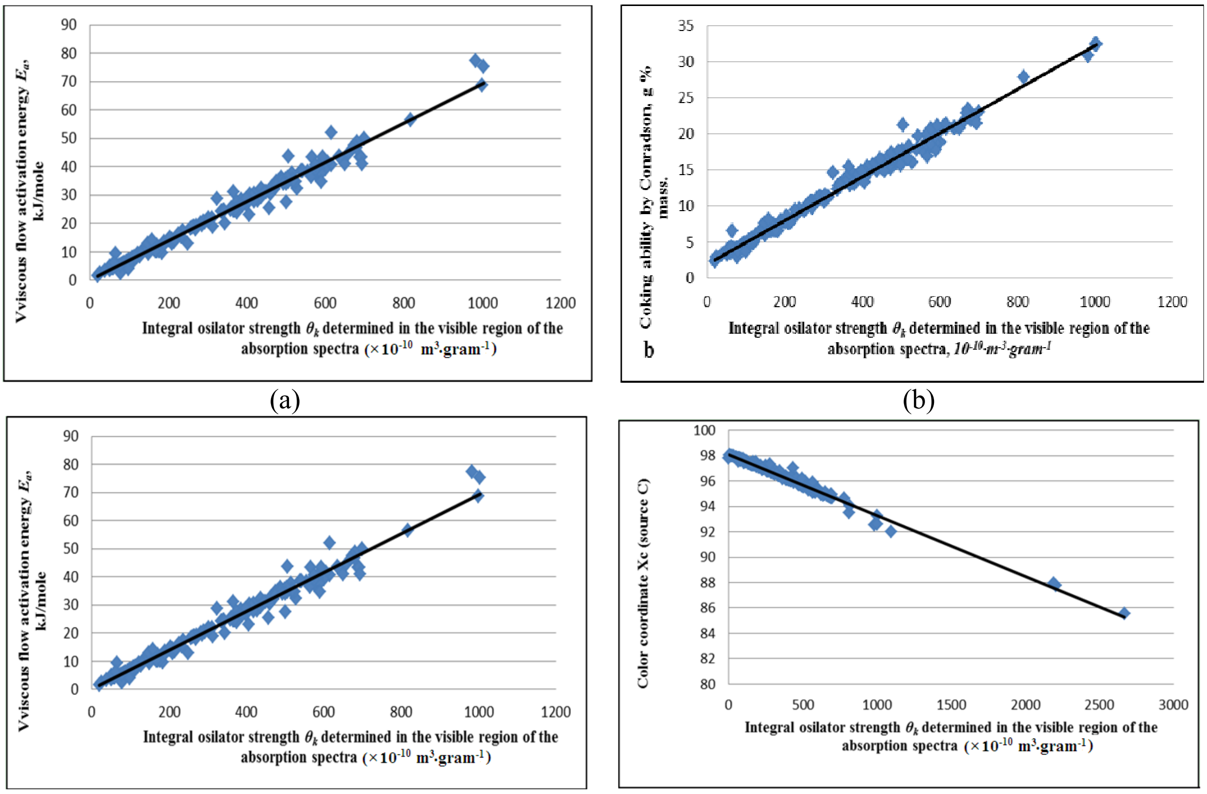


Fig. 2 Examples of absorption spectra of some multicomponent hydrocarbon systems.

Table 3 Coefficients of the Eq. (5)-(6) for different physicochemical properties of the multicomponent hydrocarbon systems.

Physicochemical property	Coefficient γ of Eq. (5)	Correlation coefficient	Variation coefficient (%)	Mean-square deviation	Fisher's ratio test for sample volume F	Table value of Fisher's ratio test F_{table}
Number-average molecular weigh W (dalton)	0.9770	0.93	13.78	82.47	1385.86	3.88
Effective IP (eV)	-0.0019	0.79	4.69	0.32	362.56	3.88
Effective EA (eV)	0.0008	0.79	10.82	0.13	362.36	3.88
Relative density (p)	0.0001	0.97	0.65	0.01	3,894.92	3.88
Initial material destruction temperature T_d (°C)	0.0915	0.93	10.28	7.70	1,385.12	3.88
Coking ability by Conradson, g % mass.	0.0303	0.99	6.45	0.74	16,772.46	3.88
Viscous flow activation energy E_a (kJ/mole)	0.0694	0.99	9.59	2.07	11,077.42	3.88
Color coordinate Xc (source C)	-0.0048	0.99	0.17	0.17	20,499.77	3.88



(a) (b)

(c) (d)

Fig. 3 Correlations between integral oscillator strength θk, determined in visible region, and different physicochemical properties of multicomponent hydrocarbon systems (222 systems): (a) number-average molecular weight; (b) coking ability by Conradson; (c) viscous flow activation energy and (d) color coordinate Xc.

- Defining of properties by the standard methods;
- Defining of absorption coefficients and IOS in the whole range of absorption;
- Calculation of coefficients of the correlations "spectrum-properties" by the least squares method according Eq. (2).

The ascertained dependences are used for defining properties on electron spectra. Atomic systems and organic π-electronic systems have been studied with this purpose. Molecular systems with aromatic connections including heteroatoms, various in their nature, have been chosen. Correlation of spectral characteristics of absorption (absorption coefficient at the fixed wavelength, (integral oscillator strength) with the following physicochemical properties have been examined: molecular weight (*W*), density (*d*), ionization potential, electron affinity (*EA*), boiling temperatures (Tb_{oil}), concentration of paramagnetic centers, coking ability by Conradson (*g*). The relative mistake of definition of properties does not exceed 10% of the property, correlation makes 0.85-0.99.

As it is shown in Table 3, the principle of interrelation of the type "spectrum-properties" is feasible for complex substances.

3. Estimation of Physicochemical Properties According to Correlaton "Property-Absorption Coeffitient"

On the one hand, it is known that the electronic structure of substances defines their physical and chemical properties, and on the other hand, their spectra.

Table 4 Coefficients of Eq. (8) for noble gases.

Physicochemical property	Analytical wave-length λ (nm)	Coefficients of Eq. (8)			
		A_0	A_1	A_2	A_3
Molecular weight M (amu)	365	178371.60	-22,6585.40	95,489.24	-13,352.51
	500	-8450.16	6398.95	-1,192.18	
Density d_r (kg/m^3)	365	7956.8420	-10,107.700	4,259.7130	-595.6541
	500	-376.3940	285.0183	-53.0990	
Boiling temperature T_{boil} (K)	500	-20,183.04	19,412.67	-5,994.72	591.30
Melting temperature T_{mel}, (K)	500	-20,732.59	20,049.56	-6,240.41	622.67
IP (eV)	490	1,998.43	-2,018.91	677.76	-74.99
EA (eV)	510	11.21	-8.48	1.54	-

Table 5 Coefficients of the Eq. (8) for organic compounds.

Physicochemical property	Analytical wavelength λ (nm)	Organic compound	Coefficients of the Eq. (8)			
			A_0	A_1	A_2	A_3
Molecular weight M (amu)	238	1	40.98	33.11	-14.90	2.25
	270	2	109.59	-87.26	52.90	-8.10
	350	3	-5,845.21	6,609.64	-2,359.53	274.85
Density d_r (kg/m^3)	240	1	0.4841	0.5660	-0.2976	0.0437
	272	2	0.8764	0.0486		
	342	3	-1.0556	1.7728	-0.3141	
	236	2	35.69	329.35	-74.63	4.42
	240	3	-475.62	845.56	-230.48	19.13
Boiling temperature T_{boil} (K)	226	1	-62,564.32	45,074.41	-10,640.84	831.06
	250	2	-6,301.05	5,013.65	-1,237.99	103.55
	346	3	-4,835.31	5,826.64	-2,003.3	223.28
Melting temperature T_{mel} (K)	298	2	221.44	115.28	-92.57	18.96
	472	3	66,657.72	-58,879.80	17,303.68	-1,673.234
IP (eV)	240	1	10.47	-1.13	-0.15	0.11
	270	2	5.75	9.95	-6.47	1.15
	356	3	11.57	-1.67	9.30 10	0.02
EA (eV)	252	3	1.27×10^5	-8.69×10^4	1.95×10^4	-1.47×10^3

1 unsaturated hydrocarbon; 2 replaced molecules of benzene series; 3 polycyclic aromatic hydrocarbons.

The correlation of the absorption coefficients with PCPs of individual substances has been found out. Particular case of the law "spectrum-properties" have been ascertained by statistical processing of data on known properties and spectra for more than 500 systems [1, 2]:

$$Z = A_0 + \sum_i A_i \cdot K_\lambda^i \tag{7}$$

where Z is the property of the system in the corresponding units of measurements; K_λ is spectral characteristics of radiation absorption by the solution of the researched sample at the certain wavelength; I is an exponent ($i = 1$ linear, $i = 2$ quadratic, $i = 3$ cubic dependence); A_0, A_i are coefficients of polynomial for the investigated series of substances.

For individual atomic and molecular substances the Eq. (7) can be expressed by a polynomial of the third degree:

$$Z = A_0 + A_1 \cdot K_\lambda + A_2 \cdot K_\lambda^2 + A_3 \cdot K_\lambda^3 \tag{8}$$

In Tables 4-5 [6-8] data processing results of dependence (8) are given for nobble gases and unsaturated hydrocarbons, replaced connections from lines of benzene and condensed aromatic hydrocarbons.

It is ascertained that for multicomponent high-molecular systems and hydrocarbon systems the dependence is:

$$Z = A_0 + A_1 \cdot K_\lambda \tag{9}$$

where Z is PCP of a multicomponent system, K_λ is radiation absorption coefficient in UV and visible region of the spectrum on analytical wavelength λ, l·g^{-1}·cm^{-1}; A_0, A_1 are the empirical coefficients weakly dependent on the chemical nature of substances, the dimensions: (property) and (property) $\times 10^{10}$ g·m^3 consequently.

Eq. (9) is given for multicomponent hydrocarbon systems for the following properties: fixed carbon coking ability by Conradson; relative density; initial material destruction temperature etc. (Table 6).

It is necessary to note that for separate oils and hydrocarbonic fractions some laws of connection of properties and absorption coefficients were earlier known [9-12]. The further works have been developed in the direction of high-molecular systems and various properties research [13-23]. In the following works [1-4] for the first time these laws were generalized as the physical law. Thus, the existence of fundamental correlation "spectrum-properties" is shown.

The research of the correlation among properties and absorption coefficients on the analytical wavelengths have been carried out according to the same scheme as for IOS.

The analytical wavelengths have been defined where the mistake of approximation was minimal. As it is shown in Table 3, the principle of "spectrum-properties" law can be used for complex substances.

During the research it has been established that to each physicochemical property some analytical wavelengths correspond, for which dependences (8, 9) are carried out with good accuracy.

IOS is a more general spectroscopic characteristic that $K(\lambda)$ and it allows to determine PCPs with better evidence, because IOS does not depend on the wavelength.

Table 6 Coefficients of Eq. (9) for hydrocarbon systems [16, 17].

Property of multicomponent system	Analytic wavelength λ (nm)	Correlation coefficients	Coefficients of Eq. (9)	
			A_0	A_1
Relative density	352	0.95	0.8982	0.0101
Coking ability by Conradson (g% mass)	455	0.91	0.02	7.30
Viscous flow activation energy E_a (kJ/mol)	476	0.98	1.04	19.88
Number-average molecular weigh W (dalton)	667	0.93	356	1033.2
Initial material destruction temperature (°C)	714	0.96	166	5.38

There is one more qualitatively new law on the integral level: so-could law color-properties , because it is known that color is also an integral (phenomena) characteristic of matter [24].

4. Estimation of Physicochemical Properties According to Color Characteristics

The relations, which exist between properties and color characteristics (CCs) of multicomponent hydrocarbon systems, have been investigated. The dependences among color coordinates (luminosity) and various physical and chemical characteristics of the investigated substances have been ascertained. The results have been confirmed by the statistical data processing.

Color coordinates of (*X*, *Y*, *Z*), coordinates of chromaticity (*x*, *y*, *z*), hue (λ) and luminosity (*L*) have been taken as color characteristics [25-26].

CCs of multicomponent hydrocarbonic systems have been determined by the technique of the International Committee on Illumination (Commission Internationale de l'Eclairage, CIE) [27] for four standard sources (illuminants) A, B, C and D_{65}. The technique, corrected for optically transparent [25] medium, has been used. Electron absorption spectra of multicomponent hydrocarbon systems have been determined in toluene solutions in the range of 380-780 nm with the use of automatic spectrophotometer. The solutions with the optical density within the limits of 0.2-0.8 have been used. For this purpose, the cuvettes with thickness of 10 mm have been used or additional dilution a solution have been carried out. Chromaticity coordinates x and y of some individual aromatic compounds are shown in Fig. 4.

By analogy with Eq. (4) linear correlation between PCPs and CCs (the law "color-properties") has been investigated as:

$$Z = B_0 + B_1 \cdot q \qquad (10)$$

where *Z* is one of physical or chemical property; *q* is the one of solution color characteristics (for example color coordinates X_j, Y_j, Z_j in the XYZ system or R_j ,G_j, B_j in the RGB system; or chromaticity coordinates x_j, y_j, z_j in the XYZ system or trichromatic coordinates r_j, g_j, b_j in the RGB system; *j*, standard light source A, B,C, or D); B_0, B_1 are the empirical constants dependent on the type of the source and the class of researched substances, dimensional properties.

The regress coefficients B_0 and B_1 have been calculated by the method of least squares. As the criterion of adequacy, the correlation coefficient *R* and the mean-square deviation have been taken. Some results of the calculations are given in Table 7. The received results show that for all the researched petrochemical systems there is correlation dependence PCP from CC [28-32].

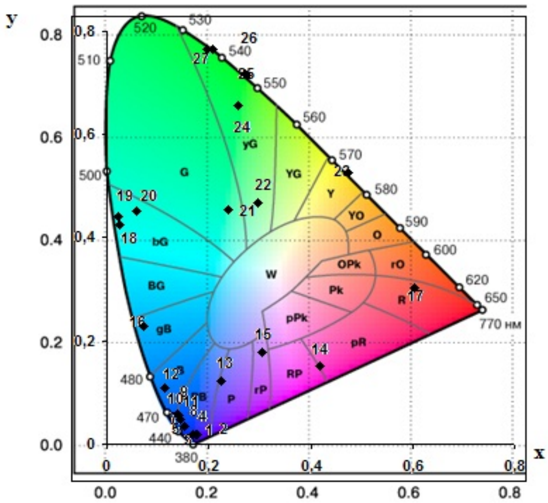


Fig. 4 Color characteristics (chromaticity coordinates x and y) of the individual aromatic oil components in XYZ colorimetric system.

(1) perylene, (2) tetrabenzpentacene, (3) dibenzpyrene, (4) hexabenzcoronene, (5) 1, 2-benzphenantrenopyrene, (6) 2, 3-benzperylene, (7) dibenzpentacene, (8) phenantrenopyrene, (9) ovalen, (10)-(12) dibenzperylenes, (13) dibenzpyrene, (14) dinaphtpyrene, (15) tetrabenzheptacene, (16) benzanathtpyrene, (17) dibenzanthanthrene, (18) bisantene, (19) benzanathtpyrene, (20) benzbisantene, (21) dinathteptacene, (22) 1, 2-benzanaphtpyrene, (23) dibenzperylene, (24) dibenzanthanthrene, (25) benzperylene, (26) dinaphtpyrene, (27) tetrabenzheptacen.

Table 7 Coefficients of Eq. (10) for physicochemical properties estimation of oils and petroleum residues in colorimetric systems XYZ and RGB [28-32].

Multicomponent hydrocarbon system	PCP	CC	Coefficients of the Eq. (10)		Correlation coefficient	Variation coefficient (%)	Fisher's ratio test for sample volume F
			B_0	B_1			
Raw oils	p	y_D	0.793	0.349	0.98	0.05	887.80
		g_A	0.758	0.310	0.98	0.05	889.46
	M	X_A	846.429	-4.563	0.99	0.48	1931.49
		R_A	897.646	-2.683	0.99	0.46	2084.20
	g	Y_B	17.063	-0.150	0.96	3.23	453.22
		R_C	17.984	-0.098	0.96	3.20	460.43
	Ea	Y_B	37.701	-0.376	0.97	5.17	536.05
		G_A	37.463	-0.140	0.97	5.16	536.51
Petroleum residues	p	x_C	0.757	0.462	0.99	0.27	577.35
		r_C	0.874	0.240	0.99	0.20	1019.05
	M	Y_B	877.611	-6.183	0.95	4.50	146.34
		r_A	-121.96	1157.340	0.96	4.31	161.29
	g	x_D	-34.205	106.697	0.98	6.80	341.48
		r_C	-6.530	53.960	0.98	5.92	455.11
	Ea	x_D	-76.698	228.968	0.98	8.31	308.21
		r_B	-22.755	110.594	0.98	7.53	378.34
Bitumens and bituminous materials	p	x_D	0.612	0.676	0.98	0.26	260.20
		r_C	0.876	0.209	0.99	0.22	384.50
	M	X_A	-11.918	1308.245	0.99	1.61	797.32
		R_A	1341.792	-6.249	0.99	1.47	958.95
	g	y_A	-570.815	255.283	0.98	3.62	252.80
		g_A	241.685	-379.399	0.98	3.64	249.38
	Ea	Y_A	-0.878	68.000	0.98	3.32	294.90
		G_A	64.355	-0.341	0.98	3.36	287.60

Table 8 Range of color characteristics of multicomponent hydrocarbon systems [33, 34].

Hydrocarbon systems	CIE standard source	Luminosity	Coordinates of chromaticity		
			x	y	z
Separator oils of the Russian Federation (Bashkortostan, West-Siberia, Tatarstan)	A	20.56-70.59	0.51-0.63	0.36-0.42	0.00-0.08
	B	17.24-66.60	0.39-0.51	0.42-0.49	0.00-0.19
	C	15.73-65.91	0.38-0.54	0.38-0.47	0.01-0.24
	D_{65}	17.17-67.42	0.37-0.51	0.39-0.50	0.01-0.23
Blown, residual, road and structural petroleum	A	9.80-64.97	0.51-0.67	0.32-0.42	0.00-0.07
	B	7.76-61.44	0.40-0.55	0.44-0.46	0.01-0.16
	C	6.60-60.88	0.38-0.61	0.38-0.43	0.02-0.22
	D_{65}	7.48-62.79	0.38-0.57	0.41-0.45	0.01-0.21
Organic fractions of oligomers	A	68.23-87.09	0.50-0.52	0.39-0.40	0.08-0.11
	B	64.75-84.41	0.36-0.38	0.39-0.41	0.20-0.25
	C	64.40-84.71	0.34-0.37	0.35-0.37	0.26-0.32
	D_{65}	65.66-85.51	0.34-0.37	0.36-0.39	0.25-0.30
Residual high-boiling hydrocarbonic fraction of vacuum oil refining	A	15.26-86.19	0.51-0.66	0.33-0.40	0.00-0.09
	B	12.15-82.06	0.38-0.57	0.42-0.47	0.01-0.20
	C	10.41-81.90	0.36-0.62	0.36-0.44	0.01-0.26
	D_{65}	11.80-83.30	0.36-0.58	0.39-0.46	0.01-0.25
Hydrocarbonic fractions with average boiling temperature T_{boil} 180-360 °C	A	21.20-99.83	0.48-0.63	0.36-0.41	0.01-0.14
	B	17.70-98.97	0.33-0.52	0.36-0.48	0.03-0.30
	C	15.98-99.96	0.31-0.55	0.32-0.45	0.04-0.37
	D_{65}	17.57-99.90	0.31-0.52	0.33-0.47	0.04-0.36
Asphaltenes and tars	A	0.10-98.67	0.29-0.86	0.14-0.41	0.00-0.33
	B	0.09-97.66	0.04-0.62	0.32-0.64	0.00-0.32
	C	0.08-98.67	0.04-0.71	0.24-0.59	0.00-0.37
	D_{65}	0.07-98.64	0.04-0.69	0.22-0.51	0.00-0.45

In Table 8, the defined CCs of multicomponent petrochemical systems are given [33, 34]. As it can be seen from the results of the calculations, CCs at the identical radiation source are close among themselves despite of their different nature. Obviously, the reason of similarity of color properties is the similarity of the absorption spectra of the systems researched. Also, the research has shown that multicomponent petrochemical systems do not have color isomerism, i.e. their CCs change depending on the radiation sources.

The specified correlations allow to determine substances PCPs with the help of CCs calculated and, on the contrary, to determine such major color characteristics as luminosity and coordinates of chromaticity with the help of PCPs. The similar correlations allow to improve the system of industrial quality of surveillance of oils and mineral oil, and also remote techniques of the control of hydrocarbonic environmental contaminations.

Table 9 Coefficients of dependence (8) for homologous series.

Dependence	$E = \alpha_1 + \alpha_2 \cdot \theta_{\lg}$					
Homologous series	IP or EA	Coefficient of correlation equations		Statistic characteristics		
		α_1, (eV)	α_2 (10^{-7}·eV·nm^{-1})	Correlation coefficient	Mean-square deviation (eV)	Variation coefficient (%)
Polycyclic aromatic compounds	IP	8.074	-0.0010256	0.76	0.22	3.07
Polycyclic aromatic compounds	EA	0.290	0.00064502	0.71	0.16	2.22
Nitrogen-containing compounds [38]	IP	10.11	-0.00250000	0.88	0.26	2.46
Oxygen-containing compounds [38]	IP	11.03	-0.00347000	0.82	0.32	2.54

Table 10 Results of investigation of linear correlation of the first ionization potential of organic semiconductors and their color characteristics [35].

Organic semiconductor class	CCs	Dependence coefficients (12) for IP		Correlation coefficients	Variation coefficients (%)	Standard deviation (eV)	Fisher's ratio test for sample volume, F	Table value of Fisher's ratio test, F_{table}	Sample volume (pcs)
		A_1 (eV)	A_0 (eV)						
Semiconductors containing three and five linear annelated benzene rings and semiconductors of perylene series	Z_C	-0.0120	8.2188	0.90	3.10	0.23	109.36	4.21	29
	Z_D	-0.0129	8.2035	0.89	3.13	0.23	106.74		
	B_C	-0.0023	8.2256	0.89	3.17	0.24	103.34		
	B_D	-0.0024	8.2110	0.89	3.20	0.24	100.79		
Semiconductor of bisantene series and anthanthrene	z_C	4.7985	3.7638	0.94	4.44	0.31	75.06	5.12	11
	z_D	4.5947	3.9328	0.94	4.47	0.31	74.09		
	b_B	4.2833	3.4563	0.94	4.71	0.32	65.89		
	b_C	5.3597	2.4476	0.94	4.52	0.31	71.99		
Semiconductors of pyrene series	x_C	-4.2636	7.8232	0.87	2.85	0.20	54.17	4.41	20
	x_D	-4.2503	7.8231	0.86	2.88	0.20	53.04		
	R_A	-0.0110	7.2866	0.87	2.86	0.20	53.91		
	R_B	-0.0148	7.3764	0.87	2.80	0.20	56.79		
Heterocyclic semiconductors	y_C	-1.9421	7.7117	0.94	1.92	0.14	93.07	4.67	15
	y_D	-1.8822	7.7100	0.93	1.96	0.14	89.11		
	g_A	-1.1612	7.5854	0.91	2.32	0.17	60.00		
	g_B	-1.2637	7.5599	0.90	2.41	0.18	54.45		

Table 11 **Results of investigation of linear correlation of electron affinity of organic semiconductors and their color characteristics [35].**

Organic semiconductor class	CCs	Dependence coefficients (12) for EA		Correlation coefficients	Variation coefficients (%)	Standard deviation (eV)	Fisher's ratio test for sample volume, F	Table value of Fisher's ratio test, F_{table}	Sample volume (pcs)
		B_1 (eV)	B_0 (eV)						
Semiconductors containing three and five linear annelated benzene rings and semiconductors of perylene series	Z_C	0.0049	0.6344	0.90	9.92	0.09	109.36	4.21	29
	Z_D	0.0053	0.6407	0.89	10.01	0.10	106.74		
	B_C	0.0009	0.6316	0.89	10.77	0.10	103.34		
	B_D	0.0010	0.6376	0.89	10.88	0.10	100.79		
Semiconductor of bisantene series and anthanthrene	z_C	-1.9716	2.4650	0.94	10.65	0.13	74.96	5.12	11
	z_D	-1.8879	2.3955	0.94	10.71	0.13	74.00		
	b_B	-1.7597	2.5912	0.94	11.29	0.13	65.68		
	b_C	-2.2019	3.0056	0.94	10.85	0.13	71.75		
Semiconductors of pyrene series	x_C	1.7519	0.7970	0.87	7.62	0.08	54.11	4.41	20
	x_D	1.7464	0.7970	0.86	7.68	0.08	52.97		
	R_A	0.0045	1.0175	0.87	7.64	0.08	53.74		
	R_B	0.0061	0.9806	0.87	7.49	0.08	56.64		
Heterocyclic semiconductors	y_C	0.7978	0.8430	0.94	5.71	0.06	93.13	4.67	15
	y_D	0.7732	0.8437	0.93	5.82	0.06	89.19		
	g_A	0.4769	0.8949	0.91	6.89	0.07	59.98		
	g_B	0.5190	0.9054	0.90	7.17	0.07	54.36		

Table 12 **Average characteristics of electron structure of the light-absorbing centers of multicomponent hydrocarbon systems [3] (Eq. (11)).**

Hydrocarbon system	EIP (eV)	EEA (eV)
Vacuum fraction of Perm oil $T_{boil} > 400$ °C	6.70	1.30
Vacuum fraction of West-Sibirean oil $T_{boil} > 400$ °C	6.32	1.41
Kushkulsk oil asphaltenes	4.7-4.9	2.1-2.15
Bronn coal asphaltenes	5.2	1.90
Oligomers such as "Asmol -1"	6.8-6.9	1.2-1.3

Table 13 **Results of ionization potential and electron affinity definition (Eq. (11)) [1, 3].**

Compounds	Ionization potential (eV)	
	EPS	Photoelectron Spectroscopy
Divinyl-butadiene 1, 3	9.08	9.07
Benzaldehyde	8.62	9.51
1, 2-Benzperiline	6.76	7.10
Coronen	7.97	7.56
	Electron affinity (eV)	
	EPS	Polarography
Anantrene	1.02	1.00
1, 2-Benzperiline	1.29	1.30
4, 5-11, 12-Dibenzoperirrene	0.94	1.10
Tetrazen	0.89	0.90

Table 14 Phenomenological parameters of the absorption spectrums of plasma subsystem for donors and four groups of patients [40, 42].

	Plasma				
	Donors	Patients			
		Pyoinflammatory desiases	Reanimation state	Renal insufficiency	Cirrhosis
Integral oscillator strength (IOS), θ (nm)					
Average value	409.2	518.8	552.9	578.49	746.6
Confidence interval $\alpha = 0.95$	21.2	28.5	39.2	29.41	61.0
Variation coefficient	24.89	21.68	23.16	17.01	16.67
Δ (nm)	-	109.6	143.7	167.2	337.4
Effective ionization potential (eV)					
Average value	8.529	8.26	8.179	8.12	7.72
Confidence interval $\alpha = 0.95$	0.503	0.067	0.093	0.08	0.15
Variation coefficient	2.95	3.24	3.72	3.14	3.84
Δ (eV)	-	-0.269	-0.35	-0.41	-0.811
Effective electron affinity (eV)					
Average value	0.51	0.617	0.651	0.686	0.84
Confidence interval $\alpha = 0.95$	0.207	0.028	0.038	0.03	0.06
Variation coefficient	20.39	27.69	29.07	15.46	19.63
Δ (eV)	-	0.107	0.141	0.176	0.33

Table 15 Parameters of identification of multicomponent systems [43, 44].

Multicomponent system	Parameters of identification		
	$\ln Q$	$P \times 10^{-3}$	$T(\lambda)$
Romaskinskaya oil	4.06	10.10	19.11
Kushkuljskaya oil	4.21	9.86	20.12
Vyatka oil	4.20	8.27	17.81
West-Siberian separator oil	9.55	8.73	10.01
Igrovskaya oil	3.90	6.26	22.81
Treated polivinilchloride	5.48	7.00	16.21
Benzine pyrolysis tar	5.45	21.77	16.31
Tar asphaltenes	6.90	9.50	6.00
Polyantracene	1.00	6.70	3.60

5. Examples for EPS Applications in Chemistry and Nanotachnology

The phenomenological approach may be used for determination of the medium indexes of reaction capability of systems characterizing its chemical activity. The average characteristic-indexes of electronic structure for the whole system were determined on the analogy with indexes of reaction capability in chemistry of “pure substances”. The problems have been solved on the basis of discovered connections between IOS (the area under the curve of absorption of radiation in visible and UV region of spectrum) and CCs with ionization potentials (IP) and electron affinity (EA). In the course of statistical research of several hundreds of atoms’ spectrums and organic molecules the correlation of IP and EA and logarithmic integral oscillator strength (LG IOS) and CCs has been ascertained:

$$E = \alpha_1 + \alpha_2 \cdot \theta_{\lg} \tag{11}$$

$$E = \beta_1 + \beta_2 \cdot q \tag{12}$$

where E is energy of the boundary molecular orbital

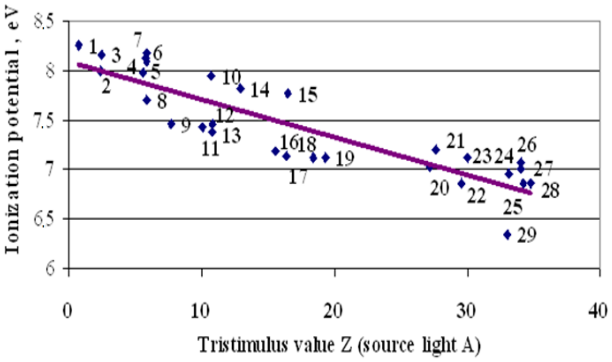


Fig. 5 The correlation of the first PI and the color characteristic for the compounds with 3 and 5 linear annulary benzene rings and from the perilene series.

(1) 2, 3-benzpizene, (2) 1, 12-2, 3-8, 9-tribenzperylene, (3) 1, 12-2, 3-dibenzperylene; (4) anthracene [2',1':1,2] anthracene; (5) coronene; (6) 2, 3-8, 9-dibenzpizene; (7) 3, 4-benzpentaphene; (8) pentaphene; (9) perilene; (10) Naphtha [2', 3':3, 4] pentaphene; (11) 1, 12-0-phenylenperilene; (12) 1, 2-benzcoronene; (13) 1, 2-3, 4-5, 6-10, 11-tetrabenzanthracene; (14) 2, 3-8, 9-dibenzpizene; (15) 1, 2-7, 8-dibenzcoronene; (16) 1,12-0-phenyl -2, 3-10, 11-dibenzperilene; (17) naphtha [2', 3':1, 2] coronene; (18) 2, 3-10, 11-dibenzperylene; (19) 2, 3-benzperylene; (20) 1, 2-3, 4-5, 6-tribenzcoronene; (21) anthracene [2', 1':1, 2]tetraphene; (22) 1, 2-benzperylene; (23) 1, 2-10, 11-dibenzperylene; (24) 1, 2-3, 4-8, 9-10, 11-tetrabenzpentazene; (25) 1, 2-11, 12-dibenzperylene; (26) 1, 2-8, 9-dibenzpentazene; (27) 1, 2-benzpentazene; (28) pentazene; (29) 1, 2-7, 8-dibenzpizene.

(IP or EA), eV; α_1, α_2 are empirically determined coefficients given in Refs. [1, 3, 35-38], eV and nm^{-1} respectively; θ_{1g} is the integral logarithmic index of absorption (logarithmic IOS), nm; $\varepsilon(\lambda)$ is the molar extinction coefficient, l·mole^{-1}·cm^{-1}; λ_1, λ_2 are borders of the spectrum in UV and (or) visible region, nm; q is one of the color characteristics; β_1, β_2 are the empirical constants dependent on the type of the source and the class of researched substances given in Refs. [35, 36, 39], dimensions of the properties. Eqs. (11) and (12) are particular cases of the dependences Eqs. (4) and (10) consequently for such properties as IP and EA. Here logarithmic IOS θ_{1g} characterizes the scale of the molecular quantum system and is used as an integral spectral characteristic Eq. (3).

Physical meaning of the dependence Eq. (11) is strong electron correlation among all the states of electrons in a molecule. This correlation is not reflected in modern methods of quantum theory in some cases.

Size θ_{1g} of this equation has weak dependence on solvent in which the spectrum is determined. Special cases of the dependence Eq. (11) for π-electronic organic systems are defined (Table 9).

Statistical processing of results shows that dependence Eq. (12) is satisfactorily carried out for different light sources and different classes of aroma compounds (Tables 10 and 11, Fig. 5).
Later, the relation (Eq. (11)) was confirmed by IP and EA for various sulfur organic compounds, nitrogen organic compounds, organic dyes, amino acids as well as biological liquids (part 6 of the review).

The determination of the electronic structure of materials and nanomaterials is a significant problem of molecular electronics. For this purpose EPS has been used. This application of EPS has been proposed in our previous works (Dolomatov at al.) [28, 35, 37].
There is a possibility of reactivity characteristics determination by electron absorption spectra for very complex, multicomponent systems. The authors have introduced some new values: effective ionization potentials (EIP) and electron affinities (EEA) [2]. They allow to estimate the electron states of multicomponent and high-molecular substances, such as heavy residual resins of oil processing, high-molecular compounds and others. In Table 12 the results of research of EIP and EEA of multicomponent hydrocarbon systems are given. From the received results it follows, that the equation is distributed to substances with IP < 9.8 eV, i.e., it covers the majority of organic substances.

IP values for simple organic molecules obtained by the dependence (11) were confirmed by various modifications of quantum semiempirical and ab-initio methods. Besides IP values have been estimated by the photoelectron spectroscopy method. The results are shown in Table 13.

Thus, it may be concluded that the Eqs. (11) and (12) allow to estimate the energy levels of quantum systems with adequate accuracy. It is important for studying many-electron systems in molecular electronics and nanotechnology, such as single molecules, atomic clusters and high-molecular systems.

From here it follows that electronic spectra can be applied to the defining of various characteristics of substances.

6. Electron Phenomenological Spectroscopy Application for Estimation of Functional State of the Human Organismic

We have examined 100 donors and 180 ailing people with different diagnosis and gravy conditions. The absorption spectra have been determined for plasma of human blood water solutions in wavelength interval from 180 to 1,080 nm with 20 nm the step. Differences between average spectra of blood components in groups of patients (with pyoinflammatory diseases, therapeutic reanimation state, with renal insufficiency and cirrhosis) and average spectra of blood components of donors especially became apparent for plasma (Fig. 6).

Integral logarithmic oscillator strength, effective (average value of all light-absorbing components) ionization potentials (EIP) and effective electron affinity (EEA) have been estimated in interval from 240 nm to 800 nm:

$$\theta_k = \int_{\lambda_1}^{\lambda_2} Lg(k(\lambda))d\lambda \tag{13}$$

$$E = \alpha_1 + \alpha_2 \cdot \theta_k \tag{14}$$

where θ_k is logarithmic IOS,·nm; $k(\lambda)$ is an absorption coefficient on wavelength λ, l·gram^{-1} cm^{-1}; λ_1, λ_2 is borders of the spectrum in UV and (or) visible region, nm; E is EIP or EEA, eV; α_1, α_2 are empirically determined coefficients given in work [40], eV and eV·nm^{-1}, respectively.

Estimated integral parameters of plasma system of human blood in conditions of homeostasis (donors) and deflections from homeostasis (patients) are presented in Table 14.

Parameters of average effective electronic structure of plasma (EIP and EEA) were calculated on the base of empiric factors, estimated for model compounds of amino acids. Evident differences may be observed for the donors and in the cases of different groups of patients.

Thus, correlation between functional state of human organism and deflection of phenomenological spectrum parameters of plasma from the homeostasis state have been determined. Most reliable results may be observed for absorption spectra of plasma in interval from 240 nm to 800 nm. It is offered to use aberrations from relative "average" standard, calculated on the basis of donors, for estimation of condition of ailing or healthy organism.

Such integral characteristic as color have been also researched in the problem of the functional state of health [41].

Phenomenological approach enables express-evaluation of the functional state of health for men with non-specific physicochemical parameters such as: IOS, EIP and EEA and some other identification parameters [40, 42].

7. Method of Complex Substances Identification on Absorption Spectra

Identification method have been offered for complex chemical systems [43]. The content of this method is approximation of spectrum by next function:

$$K = \int_{\lambda_1}^{\lambda_2} Q \cdot \exp(-p\lambda)d\lambda + T(\lambda) \tag{15}$$

where K is absorption coefficient, l·gram^{-1} cm^{-1} ; λ_1, λ_2 are borders of the spectrum; Q *is* the factor of intensity; p is probability of light absorption; $T(\lambda)$ is

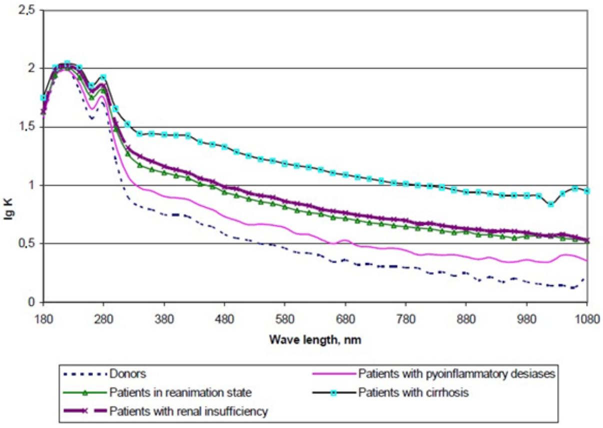


Fig. 6 Four patient groups in comparison with donors (average spectrums of plasma subsystem).

the contribution to absorption due to the effects of deviation from the exponential distributions.

The contribution of thin structure at any wavelength can be assessed as deviation (rejection) of real distribution K_p from exponential distributions K_e with the subsequent summation at all wavelengths, as it is shown:

$$T(\lambda) = \sum \frac{\left| K_{e,i} - K_{p,i} \right|}{K_{e,i}} \tag{16}$$

The integral factor of thin structure is not additive and characterizes the contribution of rotary and oscillatory conditions of various molecules to multicomponent system.

The results of the calculation of these parameters for electronic spectra in the range 300-800 nm of some typical hydrocarbon compounds, oils, mineral oil, polymers and others are given in Table 15.

The probability of light absorption p is an additive physical value. It follows from the tabulated data that the dimension of parameter p is about 10^{-3}. If to take into account the distinction of parameters of the $T(\lambda)$ and Q there are practically no two compounds with identical values of 3 parameters. Differently, these parameters are original “fingerprints” of multicomponent compounds and they can be used for identification of hydrocarbon fractions. This physical characteristic, probability of light absorption p is applied at the definition of efficiency of petroleum layers and the definitions of hydrocarbonic environmental contaminations [45, 46]. The most precise identification is expedient for carrying out in UV region of the spectra. It is shown, that the similar way is applicable for the identification of individual substances-hydrocarbons and dyes [47].

8. Conclusions

The offered methods of research of properties of simple and complex substances based on the phenomenological approach to electronic spectra of absorption and reflection when the substance is considered as integral continuous quantum system (quantum continuum of electron states).

The principle of correlation of properties and optical characteristics of absorption of substances in visible and UV, regions which is fair for any substance (correlations of type spectrum, properties and color, properties) is ascertained. The received laws are recommended for forecasting properties of organic substances, calculating them on these phenomena. The established optical laws can find use in chemical and oil engineering, medicine and nanotechnology. The phenomenological spectroscopy method will allow to define different physicochemical properties in industry and complex substances control laboratories. Besides, the definition of average properties of any substances, for example, components of cells, biopolymers, biology liquids, space objects is possible. The established laws can be used for properties estimation using reflection and absorption spectra.

It means that in visible region of the spectrum each property relates with characteristic hue. The results received mean that light radiated by the quantum continuum contain information about all properties of the matter. The task of the researcher is to use this information in the analytical purposes.

New approach developed by the group of Dolomatov can be used for investigating properties of

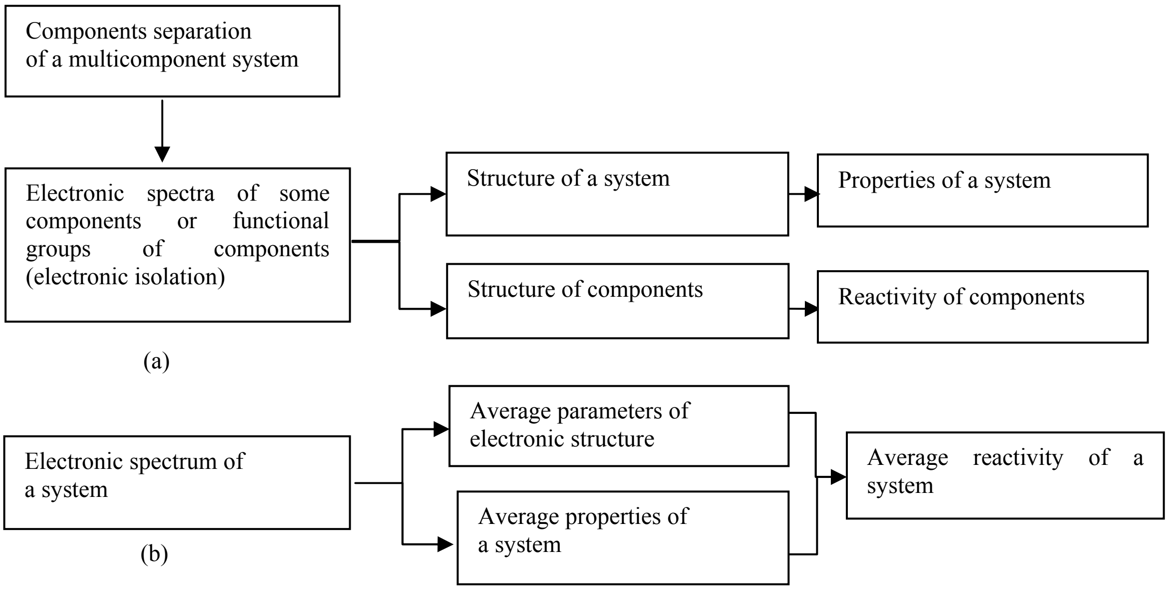


Fig. 7 Th advantages of the phenomenological approach (b) to studying of electronic spectra in comparison with the standard one (a).

the complex systems by their electron spectra. Contrary to conventional methods phenomenological spectroscopy studies substance as one indivisible system, without separating spectrum of the substance into characteristic frequencies and wavelengths of individual functional groups of components of the system. The scheme, which shows advantages of the phenomenological approach to studying of electronic spectra in comparison with the standard one, is shown in Fig. 7.

The electronic phenomenological spectroscopy is based on the correlations between integral optical characteristics and properties of substance as a single whole quantum continuum: laws "spectrum-properties" and "color-properties". According to these laws the physicochemical properties of substance solutions in UV, visible and near IR regions of the spectrum are in proportion to quantity of radiation absorbed.

Appling EPS methods one of the very important problems, the problem of prediction of the reaction capability of multicomponent substances can be solved. The phenomenological approach can be used for defining average characteristics of reactionary ability of the complex systems describing their chemical activity by analogy to the parameters of reactionary ability in chemistry of "pure substances".

The EPS methods have been developed for identification and simultaneous determination of the set of various physicochemical properties of natural and technogenic multicomponent organic systems as well as the properties of individual substances. For example, it is possible to determine in a few minutes such properties of oils as average molecular wieght, viscosity, density, the index of thermal stability, the index of reactivity of fractions in coking and thermal cracking processes, etc. The EPS methods can be used in petroleum and petrochemical industries, environmental monitoring, biophysics, medicine, criminalistics and space exploration and other.

References

[1] M.Yu. Dolomatov, Application of electronic spectroscopy in physico-chemistry of multicomponent stochastic and complex molecular system, Ufa: Center of Scientific and Technical Researches, 1989, p. 47.

[2] M.Yu. Dolomatov, Some physic-chemical aspects of prediction properties of multicomponent systems in conditions of extreme influences, Journal of D.I. Mendeleev

Russian Chemical Society 36 (5) (1990) 632-639.

[3] M.Yu. Dolomatov, Physico-chemical bases of new methods of research of complex multicomponent systems, Perspectives of practical application, Moscow, SRI for Petrochmistry, 1991, p. 72.

[4] M.Yu. Dolomatov, Fragemts of real substanse theory, From hudrocarbon systems to galaxies, Moscow, Chemistry, 2005, p. 208.

[5] M.Yu. Dolomatov, O.T. Kydyrgychova, L.A. Dolomatova, V.V. Kartasheva, Color the characteristics petrochemical systems, Journal of Applied Spectroscopy 67 (3) (2000) 387-389.

[6] G.R. Mukaeva, M.Yu. Domatov, Method for determining the ionization potential and electron affinity of aromatic compounds molecules using electron spectroscopy, Journal of Applied Spectroscopy 53 (6) (1990) 950-953.

[7] M.Yu. Dolomatov, G.R. Mukaeva, Method for determining the ionization potential and electron affinity of atoms and molecules using electron spectroscopy, Journal of Applied Spectroscopy 56 (4) (1992) 570-574.

[8] M.Yu. Domatov, G.R. Mukaeva, Application of electronic phenomenological spectroscopy for research of physicochemical properties of molecular systems, Oil Refining and Petrochemistry 1 (1995) 22-26.

[9] I.L. Marhasin, Physico-chemistry of the mechanics of a petroleum layer, M.: Bowels, 1974, p. 100.

[10] Z.F. Kuz'mina, R.S. Sarmanaev, M.F. Galiakbarov, R.M. Usmanova, A.F. Ahmetov, R.B. Vahitov, Optical density as a parameter of carbon forming abilities of gasolines, Oil Refining and Petrochemistry 11 (1979) 14-15.

[11] Z.F. Kuz’mina, Research by spectral methods distillate and residual mineral oil, as raw material of thermal processes, Ph.D., Thesis, Ufa, Ufa Oil Institute, 1980. p. 25.

[12] Z.F. Kuz'mina, A.A. Bajbazarov, S.M. Slutskaja, L.V. Krasnova, Way of definition of an output of coke from the petroleum rests, USSR Patent 864071 (1977).

[13] M.Yu. Dolomatov, Chemical Physics of Multicomponent Organic Systems, Russia, Ufa Institute of Petroleum Refining and Petrochemistry, 2000, p. 122. (book)

[14] Works of the first Russian scientific seminar on coloristic and electronic spectroscopy of complex systems Information-Color-Property, Russia, Ufa, Technological Institute of Service (1998) 44p.

[15] M.Yu. Dolomatov, G.R. Mukaeva, Application of phenomenological electronic spectroscopy for molecular systems physicochemical properties analysis, Oil Refining and Petrochemistry 5 (1995) 22-26.

[16] M.Yu. Dolomatov, Thermodynamic analysis of correlations spectrum-properties in complex molecular and multicomponent systems, Bashkir Chemical Journal 17 (3) (2010) 75-80.

[17] G.R. Mukaeva, Forecasting of physical and chemical properties of individual hydrocarbons and petroleum disperse systems with the help of electron spectroscopy, Thesis, Ph.D., Tomsk: Siberian Branch of Russian Academy of Sciences, Institute of Petroleum Chemistry . 1997, p. 25.

[18] L.M. Hasper, Definition of rheological characteristics of petroleum disperse systems with application of radiospectral methods and electronic spectroscopy, Ph.D. Thesis, Tomsk: ICC COAC the Russian Federation, 1998, p. 25.

[19] M.Yu. Dolomatov, Z.F. Kuz’mina, S.P. Lomakin, L.M. Hashper, Express of definition of relative density petroleum’s fraction, Chemistry and Technology of Fuel and Oils 9 (1991) 32-34.

[20] M.Yu. Dolomatov, L.M. Hashper, Z.F. Kuz’mina, Spectroscopic method of definition of average molecular weight, Chemistry and Technology of Fuel and Oils 7 (1991) 34-35.

[21] M.Yu. Dolomatov, L.M. Hashper, Spectroscopic way of definition of energy activation viscous’s current of mixes high-molecular organic connections, Oil Refining and Petrochemistry 10 (1990) 38-41.

[22] M.Yu. Dolomatov, Z.F. Kuz’mina, S.P. Lomakin, L.M. Hasper, Definition mixes of coking ability high-molecular organic connections, Chemistry and Technology of Fuel and Oils 9 (1991) 29-30.

[23] M.Yu. Domatov, Application of electronic phenomenological spectroscopy for identification and research of complex organic systems, Chemistry and Technology Fuels and Oils 1 (1995) 29-32.

[24] M.D. Fairchild, Color Appearance Models, Second Edition, Wiley-IS&T Series in Imaging Science and Technology, Chichester, UK, 2005.

[25] Application of coloristic in the textile industry, Part 1, 2nd ed., USSR, Moscow, 1971, p. 400.

[26] Methods of research in textile chemistry, G.E. Krichevsskogo’s ed., Light sindustrial publishers, Moscow, 1993.

[27] ISO/CIE 10526, CIE Standard Illuminants for Colorimetry.

[28] M.Yu. Dolomatov, D.O. Shulyakovskaya, G.R. Mukaeva, N.Kh. Paymurzina, Testing amorphous, multi-component, organic dielectrics according to their electronic spectrums and color charcteristics, Applied Physics Research 3 (2012) 83-87.

[29] M.Yu. Dolomatov, G.U. Jarmuhametova, Number-average molecular weigh definition of oils and petroleum residues by color characteristics, Chemistry and Technology Fuels and Oils 4 (2009) 46-49.

[30] M.Yu. Dolomatov, G.U. Jarmuhametova, Calculation of average molecular mass, cocking capacity and viscous flow activation energy of oil surface samples by color-properties correlations, Geology, Geophysics and Reservoir Engineering 7 (2009) 35-38.

[31] M. Yu. Dolomatov, G.U. Yarmukhametova, Correlation of color characteristics with conradson carbon residue and molecular weight of complex hydrocarbon media,

Journal of Applied Spectroscopy 75 (3) (2008) 433-437.

[32] M.Yu. Dolomatov, G.U. Jarmuhametova, L.A. Dolomatova, The interaction of color and physicochemical properties of hydrocarbon systems in colorimetric systems RGB and XYZ, J. Applied Physics 4 (2008) 43-49.

[33] M.Yu. Dolomatov, V.V. Kartasheva, J.G. Ponomareva, Definition physicochemical characteristics of complex hydrocarbonic systems on correlations color-property, Oil Refining and Petrochemistry (Scientifically-Practical Conference) 5 (2002) 262-268.

[34] M.Yu. Dolomatov, G.U. Jarmuhametova, The nature of the color and color characteristics of multicomponent hydrocarbon systems, Bashkir Chemical Journal 4 (2009) 62-68.

[35] M.Yu. Dolomatov, D.O. Shulyakovskaya, G. R. Mukaeva, G.U. Jarmuhametova, K.F. Latypov, Simple characteristics estimation methods of material and molecule electronic structure, Journal of Materials Science and Engineering 5 (2012) 261-268.

[36] M.Yu. Dolomatov, G.R. Mukaeva, G.U. Jarmuhametova, D.O. Shulyakovskaya, Simple definition methods of electron structures of materials and molecules for nanoelectronics, Nanotech Europe, Berlin, Germany, 2009. p. 172. http://www.nanotech.net/content/conference/abstract-submission/simple-definition-methods-electron-structures-materials-and-m

[37] M.Yu. Dolomatov, D.O. Shulyakovskaya, G.U. Jarmukhametova, Fenomenological spectroscopy estimation methods of electron structures moleculas for electronics, ELECMOL'10, in: 5th International Meeting on Molecular Electronics, Grenoble, France, 2010, p. 255.

[38] K.F. Latypov, M.Yu. Dolomatov, Defining the first adiabatic ionization energy of the molecules of the oxygen-containing and the nitrogen-containing substances by integral characteristics of electronic spectra, Bashkir Chemical Journal 19 (1) (2012) 144.

[39] M.Y. Dolomatov, G.U. Jarmuhametova, D.O. Shulyakovskaya, The estimation of the first ionization potentials and electron affinity of the molecules of polycyclic organic semiconductors applying the color characteristics in colorimetric systems XYZ and RGB, Journal of Applied Physics 1 (2011) 20-31.

[40] M.Yu. Dolomatov, N.V. Kalashchenko, T.R. Arslanov S.V. Dezortsev, Spectroscopic phenomenologycal estimation of the functional state of human organism in rate and pathology, International Journal of Clinical Medicine 2 (2011) 79-81.

[41] M.Yu. Dolomatov, N.V. Kalashchenko, S.V. Dezortsev, T.R. Araslanov, Features of color characteristics of blood plasma of patients with liver cirrhosis in the colorimetric system XYZ as compared with healthy people, International Journal of Clinical Medicine 3 (3) (2012) 211-214.

[42] N.V. Kalashchenko, M.Yu. Dolomatov, S.V. Dezortsev, The electronic phenomenological spectroscopy blood of human in rate and pathology, Theory and Practice Aspects: Moscow: Inter., (2010) 256.

[43] M.Yu. Dolomatov, L.A. Dolomatova, P.P. Muravjev, Definition of a nature of multicomponent mixes on integral spectral characteristics, Journal of Analitical Chemistry 47 (8) (1992) 1300-1303.

[44] M.Y. Dolomatov, L.A. Dolomatova, Z.F. Kuz'mina, Method of identification of spectra of multicomponent natural and technological systems, Journal of Applied Spectroscopy 55 (3) (1991) 369-374.

[45] M.Yu. Dolomatov, L.A. Dolomatova, P.P. Muravjev, Z.F. Kuz'mina, A way of oils and mineral oils identification, Patent, A.C.USSR, 1552081 (1989).

[46] L.A. Dolomatova, M.Yu. Dolomatov, A.G. Telin, N.I. Hisamutdinov, Spectroscopic way of identification oil's, Oil Refining and Petrochemistry 1 (1998) 21-23.

[47] L.A. Dolomatova, O.T. Kydyrgycheva, M.Yu. Dolomatov, Method of identification of petrochemical systems and individual substances, Oil Refining and Petrochemistry 12 (1997) 19-22.