

Testing Amorphous, Multi-component, Organic Dielectrics According to Their Electronic Spectrums and Color Characteristics

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Abstract

The original methods of determining physicochemical properties (e.g. relative density, fixed carbon coking ability, viscous flow activation energy, number-average molecular weight, initial material destruction temperature) and characteristics of electronic structure (ionization potentials and electron affinity) of hydrocarbon systems were generalized. In the considered methods for testing dielectrics based on these systems named characteristics are estimated according to radiation absorption coefficients, color characteristics of substance solutions and integral oscillator strength in visible and UV spectrum region. The proved regularities are confirmed with statistical processing of data.

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1. Introduction

Many dielectrics, which are used in electrical engineering are created on the basis of hydrocarbon multi-component disperse systems, including bitumens, bitumen-polymer compositions, hydrocarbon oils and etc. The amorphous and viscous flow state, chaos and multi-component composition (Pecheny, 1990) are typical properties for these systems at operation temperatures. There arises a problem to perform a quick testing of physicochemical properties (PCP) during the exploitation of such dielectrics. It is quite difficult to test hydrocarbon systems (HCS) using conventional methods since they include a great number of interacting components, whereas the existing methods are time-consuming. This was the reason why express methods of PCP testing were introduced, which incorporate a number of new physical regularities.

2. Estimation of Physicochemical Properties according to the Radiation Absorption Coefficients

In previous investigations we managed to determine that there are correlations between optical characteristics and PCP, including HCS for compositions named as a spectrum-property correlation (Mukaeva, Dolomatov, 1998, p438-440; Dolomatov, 2005) ("spectrum-properties" law):

$$Z = A + B \cdot K_{\lambda} \quad (1)$$

where Z is one of the HCS physicochemical properties; K_{λ} is the radiation absorption coefficient of substance solution with the wave length λ (wave length λ is in the area of visible and closest ultraviolet/infrared spectrum regions). In general case K_{λ} is integral oscillator strength (dependence (3)), which define all equilibrium physicochemical properties of solution (Dolomatov, 2005), (Dolomatov, 2000); A , B are empirical coefficients, determined with physicochemical properties, nature of investigated systems, including electromagnetic spectrum range.

3. Estimation of Physicochemical Properties according to the Color Characteristics

Further investigations (Dolomatov, Kydyrgycheva, Dolomatova, & Kartasheva, 2000, p387-389) showed that a linear correlation between PCP and color characteristics (CCs) of substance solutions in optically transparent solvents is performed as the following correlation ("color-properties" law):

$$Z = B_0 + B_1 \cdot H \quad (2)$$

where Z is a physicochemical property; H is one of the color characteristics of solutions, e.g. lightness, color coordinates; B_0 , B_1 are constants depending on a property such as a radiation source and nature of investigated substances.

Electron absorption spectrums of hydrocarbon, multi-component dielectrics and aroma solvents (bitumens, tars and asphaltene materials, light and heavy hydrocarbon fractions – 100 dielectrics in total) are used as subjects for investigation. CCs - color and chromaticity coordinates in systems XYZ and RGB (ISO/ CIE 10526), including color lightness were determined according to transmission factor of organic dielectric solution in the visible spectrum region for four standard sources of visible radiation A, B, C and D₆₅ (Fairchild, 2004). Then applying the method of least squares a linear correlation between PCP and CCs of different systems was tested. This work provides a description of substance correlation with the following color characteristics for sources A, B, C и D₆₅: $x_A, y_A, z_A, x_B, y_B, z_B, x_C, y_C, z_C, x_D, y_D, z_D$ - chromaticity coordinates in the XYZ system; $X_A, Y_A, Z_A, X_B, Y_B, Z_B, X_C, Y_C, Z_C, X_D, Y_D, Z_D$ - color coordinates in the XYZ system; $r_A, g_A, b_A, r_B, g_B, b_B, r_C, g_C, b_C, r_D, g_D, b_D$ - trichromatic coordinates in the RGB system; $R_A, G_A, B_A, R_B, G_B, B_B, R_C, G_C, B_C, R_D, G_D, B_D$ - color coordinates in the RGB system.

Statistical criteria of accuracy and regression coefficients for (2) for bituminous materials are shown in Table 1.

Table 1. Testing physicochemical properties of multi-component organic dielectrics according to dependence (2)

Dielectrics	PCP	CCs	Regression coefficient		Correlation coefficients, R	Variation coefficients, %	Fisher's ratio test, F_{design}
			B_0	B_1			
Bituminous materials	relative density, ρ	b_C	0.9451	-0.1454	0.97	0.30	189.36
	fixed carbon coking ability g , weight %	g_A	83.24	-117.37	0.98	3.62	252.63
	viscous flow activation energy E_a , kJ/mole	b_B	12.52	-92.95	0.97	4.20	177.42
	initial material destruction temperature T_d , °C	X_A	121.16	-1.16	0.99	1.60	509.75
	number-average molecular weigh W , mole	B_A	1151.25	15.07	0.99	1.50	866.47

Figure 1 shows data on testing viscous flow activation energy of electroinsulating and construction bitumens according to color characteristics.

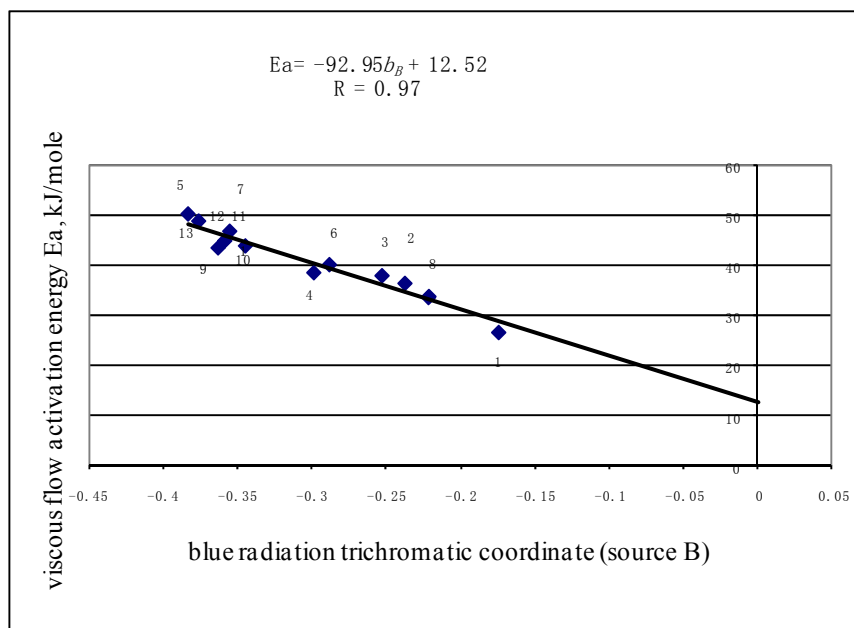


Figure 1. Viscous flow activation energy of bituminous dielectric materials as a function of blue radiation trichromatic coordinate (source B)

Points 1-4 residual bitumen; 5- air-blown bitumen (melting point T_m acc. to ring-and-ball test 86 ° C); 6- bitumen from the composition of Siberian oils (melting point T_m acc. to ring-and-ball test 38 ° C); 7- compounded bitumen (melting point T_m acc. to ball-and-ring test 60,5 ° C); 8- residual bitumen from Arlan oil; 9- low-melting penetration isolating bitumen; 10- high-melting air-blown bitumen from West Siberian oil; 11- air-blown bitumen from gas pyrolysis tars; 12- air-blown eclectic cable bitumen from West Siberian oil; 13- high-blown electroinsulating bitumen.

4. Estimation of Ionization Potentials and Electron Affinity According to the Integral Oscillator Strength in the Electronic Absorption Spectrum

Among one of the most important properties of solids are average properties of band structure. The previous tests suggest a determination of ionization potential (IP) and electron affinity (EA) on empirical dependences, which correlate these properties with the integral absorption coefficient θ , which is in fact analogous of integral oscillator strength ($\theta \rightarrow$ IOS) (Dolomatov, Shulyakovskaya, Mukaeva, Jarmukhametova, Latypov, 2012, 261-268). In the course of statistic investigating some hundreds of atom and molecule spectrums on PCs the detected regularities were confirmed with the satisfactory accuracy with the mean error 0.1-0.2 eV (Dolomatov, Mukaeva, 1992, 570-574), (Dolomatov, Shulyakovskaya at al. 2009, 172), (Dolomatov, Shulyakovskaya, Jarmukhametova, 2010, 255). The dependence is as follows («spectrum-properties» law):

$$E = \alpha_1 + \alpha_2 \cdot \int_{\lambda_1}^{\lambda_2} \lg \varepsilon(\lambda) d\lambda, \quad (3)$$

where E – energy of boundary orbitals, eV; α_1 , α_2 – coefficients, specified in work (Dolomatov, 2000), eV and $\text{eV} \cdot \text{mole} \cdot \text{cm}^{-1} \cdot \text{nm}^{-1}$ correspondingly; λ_1 , λ_2 – spectrum boundaries in UV – and (or) visible region, nm; $\varepsilon(\lambda)$ – molar coefficient of substance absorption, $\text{l} \cdot \text{mole}^{-1} \cdot \text{cm}^{-1}$.

Consequently, this dependence was confirmed for different IP and EA of sulphur organic compounds, nitrogen pigments, organic pigments, aminoacids and biological fluids. This dependence is used by authors to estimate ionization energy and band width of different dielectrics. Band width was approximately estimated as the difference of effective IP and EA ($\Delta E = \text{IP} - \text{EA}$), Fermi level was approximately estimated as $E_F = \Delta E / 2$. Table 2 shows the results for certain dielectrics.

Table 2. Effective parameters of multi-component dielectric band structure

Multi-component amorphous liquid dielectrics	Parameters of electronic structure		Effective band width	Fermi level
	<i>Effective ionization potential, eV</i>	<i>Effective electron affinity, eV</i>	$\Delta E, eV$	E_F, eV
Tar oil	6.420	1.410	5.050	2.525
Dielectrical oil	7.472	0.943	6.529	3.265
Electric cable bitumen from West Siberian oil	6.679	1.269	5.410	2.705
Penetration, isolating bitumen	7.126	1.085	6.041	3.021
Bitumen grade BN-3	6.653	1.280	5.373	2.687

5. Conclusions

The results are confirmed with quantum calculations for model molecule fragments of organic substances (Dolomatov, Dezortsev, Svetlana, & Shutkova, 2012, p151-157). It is indicated that a great contribution is made by free radicals of alphaltic-resinous substances, which ionization potential is approximately 1.5 eV lower and electron affinity is 1 eV higher than regular molecular fragments. Such correlations allow improving the quality control system of multi-component dielectrics in the process of their production and operation. In particular, on the basis of regularities (1-3) methods of determining the total of basic PCP of amorphous hard and viscous flow dielectrics according to CCs and characteristics of their solution absorption. Determining the properties is much quicker when using color comparators and automatic spectrophotometers. The suggested designed methods allow to determine the total of practically important properties of these materials for some minutes.

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