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ENERGY STRUCTURE OF THE LONG-WAVELENGTH ABSORPTION SPECTRA EDGE AND ITS RELATIONSHIP TO THE URBACH ENERGY E_u AND THE OPTICAL BAND GAP E_g OF C_{60} FILMS WITH THICKNESSES OF 5000 AND ∼1000 nm

The long-wavelength edge of the absorption spectra of C_{60} films with a thickness of 5000 and ∼1000 nm in the regions of 1.414–1.998 eV and 1.448–2.371 eV, respectively, was approximated by the sum of Gaussian functions (Gaussians). In C_{60} films with a thickness of 5000 nm, this edge is formed by the sum of Gaussians centered at 1.829 and 2.026 eV, whereas in C_{60} films with a thickness of ∼1000 nm, it is formed by the sum of Gaussians centered at 1.800, 1.894, 2.025 and 2.382 eV. The main contribution to the absorption of C_{60} films with thickness of 5000 nm is provided by the Gaussian centered at 2.026 eV, whereas in in C_{60} films with thickness of ∼1000 nm – by Gaussians centered at 1.894, 2.025, and 2.382 eV. The E_u values vary within the ranges of 12.15–47.69 meV and 28.04–108.44 meV, and E_g – within the ranges of 1.653–1.718 eV and 1.524–1.769 eV in C_{60} films with a thickness of 5000 and ∼1000 nm, respectively.

Keywords: film, absorption spectrum, C_{60} and C_{70} fullerenes, approximation, Gaussian function, Gaussian.

1. Introduction

The C_{60} and C_{70} fullerene molecules, discovered in 1985 [1], are closed clusters with I_h and D_{5h} symmetry and are close in shape to a sphere and a rotational ellipsoid, respectively.

In the process of fullerene synthesis, molecules with different numbers of carbon atoms are formed. The main components of this mixture are the most stable fullerene molecules C_{60} and C_{70}. Moreover, the synthesized C_{60} and C_{70} are considered to be mixtures of C_{60}/C_{70} or C_{70}/C_{60}, where the first and second components represent the main substance and the principal impurity, respectively [2]. The dynamics of changes in the composition of C_{60}/C_{70} films during their thermal deposition in vacuum was studied in [3].

C_{60} has been used in solar cells [4], photovoltaic devices [5], photocatalysts [6], phototherapy [7], and biosensors [8]. The absorption edge of C_{60} films is similar to that of films based on amorphous Si (*a*-SiC and *a*-Si: H). E_g and E_u of the C_{60} films are 1.64 eV and 61 meV, respectively [9, 10].

Under external pressure, the intensity of the absorption edge increases and it undergoes a red shift in polycrystalline granules of the C_{60}/C_{70} mixture. Moreover, the value of E_g decreases and approaches zero at a pressure of 20.5 GPa. After the pressure is re-

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moved, the absorption edge of these granules recovers its original shape, indicating that the C_{60} and C_{70} molecules remain intact. It is assumed that at pressures ≥20.5 GPa, C_{60}/C_{70} granules may exhibit metallic conductivity [11].

Depending on the temperature, there are three structural phases of C_{60} films: phase 1 (orientationally frozen phase) ($T \leq 150$ K); phase 2 (orientationally disordered phase) ($150 < T \leq 260$ K) and phase 3 (free rotation of C_{60} molecules) ($260 < T < 470$ K). Moreover, the values of E_g and E_u of C_{60} films with a thickness of 1.0–8.5 μm do not change in phase 1 and change slowly in phase 2 and rapidly in phase 3. In phases 2 and 3, with increasing temperature of the 8.5 μm thick C_{60} film, the E_g value decreases from 1.7 to 1.6 eV, whereas the E_u value increases within 30–59 meV, respectively. The E_u value strongly depends on the orientational disorder of C_{60} molecules, while O_2 intercalation does not change it, i.e., the E_u tail parameter is an intrinsic characteristic of C_{60} films [12]. Comprehensive optical and electron microscopic studies have shown that polycrystalline C_{60} films have a fundamental absorption edge near 1.65 eV and that the dependence of E_g on the mechanical stress P is $(dE_g/dP) = -2.8 \times 10^{-10}$ eV/Pa. In amorphous C_{60} films, the mechanical stress decreases and their absorption edge is located near 2.2 eV [13].

For the first time, the absorption edge was investigated and the values of E_g and E_u of submicrometer-thick C_{60} and C_{70} films with a thickness of 20–900 nm were determined [14, 15]. Similar studies were conducted for C_{60} and C_{70} films in an wider thickness range from 20 to 5000 nm [16]. In these studies, it was found that E_u decreases, whereas E_g increases with increasing film thickness for both C_{60} and C_{70} films.

Therefore, the data presented above in [9–16] indicate that the E_u and E_g values of C_{60} films depend on external pressure, temperature, and film thickness. Furthermore, the energy structure of the long-wavelength absorption edge of these films suggests that its contour is formed by several electronic transitions. The energy structure of this absorption edge has been scarcely studied in the literature.

These studies are important because the value of E_u determines the steepness of the long-wavelength absorption edge and is necessary to assess the degree of structural order of C_{60} films, which is due to the electronic states of defects in the band gap. The value of E_g makes it possible to estimate the absorption threshold of these films, which is very important for determining the efficiency of converting light energy into electrical energy in solar cells and other similar devices based on heterostructures (HS) containing C_{60} layers and C_{60} composites with various p-type semiconductors.

In Refs. [14–16], it is assumed that the energy structure of the long-wavelength absorption edge of C_{60} films with a thickness of ∼1000 nm, which was first described in Ref. [9], may be due to the vibronic progression of the triplet exciton. This assumption should be considered one possible explanation for the nature of the energy structure, since the shape of the long-wavelength absorption edge of C_{60} films can also be influenced by fullerene impurities C_n ($n > 60$) formed during the synthesis process [2]. This indicates the need for a more detailed study of the energy structure of this edge in order to identify the influence of other electronic transitions of C_{60} on its shape, including electronic transitions of possible fullerene impurities, especially C_{70}. The long-wavelength absorption of this impurity is significantly stronger than that of the original substance C_{60} [17].

In view of the above, the aim of this work is to study the energy structure of the long-wavelength edge of C_{60} films with thicknesses of 5000 and ∼1000 nm, in which this structure may be more clearly resolved than in submicrometer-thick C_{60} films. In addition, the values of E_u and E_g for the electronic transitions that form the long-wavelength absorption edge of C_{60} films with thicknesses of 5000 and ∼1000 nm will be determined. This work is a continuation of our previous studies [14–16].

2. Technology of Fabrication of C_{60} Films with Thicknesses of 5000 and ∼1000 nm

In [12], the starting C_{60} powder with a purity of 99.98% was preheated at 250 °C for 8 hours to remove O_2 and toluene. Films with a thickness of 5000 nm were obtained by thermal deposition of this powder onto glass and quartz substrates in a vacuum of 5×10^{-6} Torr with evaporator and substrate temperatures of 400 and 250 °C, respectively. After deposition, the substrates with the films were cooled to room temperature. Polycrystalline C_{60} films with crystallites 30–47 nm in size were obtained.

In [9, 10], films with a thickness of ∼1000 nm were deposited by thermal deposition of C_{60} powder onto glass substrates in a vacuum of $\sim 10^{-6}$ Torr. The C_{60} powder was pre-purified by crystallization from a solution in toluene and subsequent column chromatography. Analysis of the resulting films by mass spectrometry and Raman spectroscopy showed that these films consist almost entirely of C_{60} molecules.

3. Methods for Determining the Value of the Urbach Energy E_u and the Optical Band Gap E_g of Semiconductors

The Urbach absorption tail of semiconductors (including C_{60} films) can be described by the following relation [18]:

$$\alpha = \alpha_0 \exp\left(\frac{E - E_g}{E_u}\right), \tag{1}$$

where α_0 is a constant (measured in cm^{-1}); E is the photon energy; E_g and E_u are the optical band gap and Urbach energy, respectively.

After taking the logarithm of Eq. (1), the difference between the two $\log\alpha$ values is equal to: $\log\alpha_2 - \log\alpha_1 = ((E_2 - E_1) \times \log e)/E_u$. Let $\log\alpha_2 - \log\alpha_1 = \Delta(\log\alpha)$ and $E_2 - E_1 = \Delta(E)$. Because $\log e \approx 0.4343$, then $\Delta(\log\alpha) \approx (0.4343 \times \Delta(E))/E_u$ and $E_u \approx 0.4343/\kappa_u$, where $\kappa_u = \Delta(\log\alpha)/\Delta(E)$ is the tangent of the slope of the graph $\log\alpha = f(E)$ to the abscissa axis E.

From the above, we obtain the following expression for the value of E_u (in meV):

$$E_u \approx \frac{434,3}{k_u}, \tag{2}$$

where the coefficient k_u is measured in eV^{-1}.

To describe the absorption edge associated with indirect electronic transitions in amorphous semiconductors, the relation first established by Tauc for amorphous germanium films is used [19]. In its modern form, this relation is expressed as [16]:

$$(\alpha \times E)^{0.5} = A_2 \times (E - E_g), \tag{3}$$

where A_2 is a constant numerically equal to the tangent of the angle between the graph and the horizontal photon-energy axis E; E_g is the optical band gap.

Let $y = (\alpha E)^{0.5}$ and $A_2 = k_g$. Then Eq. (3) takes the form: $y = k_g (E - E_g)$. After rearrangement, we obtain the following expression for E_g:

$$E_g = E - \frac{y}{k_g}, \tag{4}$$

where E and y are the abscissa and ordinate of the points on the straight-line section of the graph described by Eq. (3). E_g and E are measured in eV, whereas y and the coefficient k_g are measured in $(\mathrm{cm}^{-0.5} \cdot \mathrm{eV}^{0.5})$ and $(\mathrm{cm}^{-0.5} \cdot \mathrm{eV}^{-0.5})$, respectively.

From Eq. (4) it follows that at the ordinate $y = 0$ the abscissa $E = E_g$. Therefore, the value of E_g can be determined in two ways. The first (calculated) method consists in calculating the value of E_g using Eq. (4) for the coordinates $(E; y)$ of points selected on the straight-line section of the graph described by Eq. (3). In the second (graphical) method, the value of E_g is determined by extrapolating the straight-line section of the graph described by Eq. (3) to $y = 0$.

4. Long-Wavelength Absorption Edge of C_{60} Films with Thicknesses of 5000 and ∼1000 nm

The original absorption spectra of C_{60} films with a thicknesses of 5000 and ∼1000 nm were measured by photothermal deflection spectroscopy in the photon energy range of 0.8–2.5 eV and are represented by the functions $\log\alpha = f(E)$ [12] and $\log D = f(E)$ [9], where $\log\alpha$ and $\log D$ denote the decimal logarithms of the absorption coefficient α and the optical density D of C_{60} films; E is the energy of the photons incident on the film surface.

In this work, after processing using the Origin computer program, the resulting absorption spectra $D = f(E)$ (Fig. 1, *a*) and $\alpha = f(E)$ (Fig. 1, *b*) were obtained in the photon energy ranges E corresponding to the original absorption spectra: 1.414–1.998 and 1.448–2.371 eV for C_{60} films with thicknesses of 5000 and ∼1000 nm (curves *1* and *2*, respectively).

Optical density D or absorbance A characterizes the degree of light absorption in a C_{60} film and is measured in arbitrary units (a.u.). Transmission is defined as $T = I/I_0$, where I_0 is the intensity of light incident on a C_{60} film; I is the intensity of light passing through the film. For low scattering, the optical density is given by $D = -\log T$. The upper measurement limit of D_b of most spectrophotometers is in the range of 3 to 4 a.u., which corresponds to T_b values ranging from 0.1 to 0.01%, respectively.

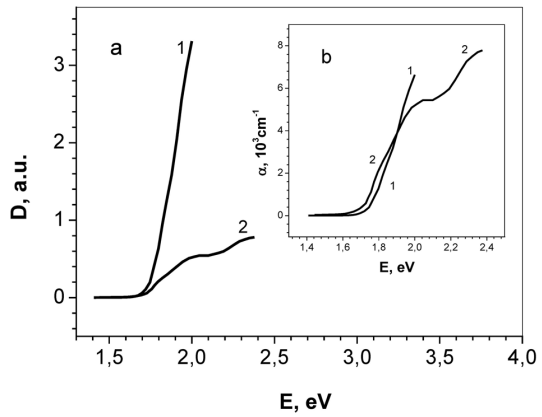

Fig. 1. Output spectra: optical density D (*a*); absorption coefficient α of C_{60} films with a thickness of 5000 nm (curve *1*) and ∼1000 nm (curve *2*) (*b*). Curves *1* and *2* are obtained from the original spectra [12] and [9], respectively

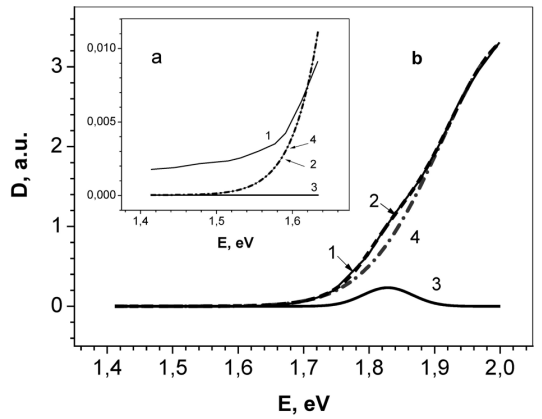

Fig. 2. Approximation by the sum of Gaussian functions of the long-wavelength edge of the absorption spectrum of a C_{60} film with a thickness of 5000 nm in the energy region: 1.414–1.633 eV (*a*); 1.414–2.026 eV (*b*). Curves *1* and *2* (solid and dashed lines), *3* and *4* correspond to the output spectrum and the summary spectrum, Gaussians centered at 1.829 and 2.026 eV, respectively

The value of the ordinate of the endpoint $D = 3.2965$ a.u. of the C_{60} film with a thickness of 5000 nm (Fig. 1, *a*, curve *1*) is the upper limit of D_b measurable with spectrophotometers without distorting the measured value. The abscissa E of the endpoint, 1.998 eV is close to the energy of 1.999 eV of the singlet $A_g \to 1T_{1g}$ transition of C_{60} films [3] and [17]. The ordinate D_0 of the starting point of this spectrum is 1.777×10^{-3} a.u. The ordinates D_0 and D of the starting and ending points of the absorption spectrum of the C_{60} film with a thickness of ∼1000 nm are equal to 3.552×10^{-3} and 0.777 a.u., respectively (Fig. 1, *a*, curve *2*). The graphs of the spectra $\alpha = f(E)$ of C_{60} films intersect at $E = 1.903$ eV and $\alpha = 3914$ cm^{-1} (Fig. 1, *b*). The spectrum of a C_{60} film with a thickness of ∼1000 nm lies above and below the spectrum of a C_{60} film with a thickness of 5000 nm for $E < 1.903$ eV and $E > 1.903$ eV (Fig. 1, *b*, curves *1* and *2*, respectively).

5. Energy Structure of the Long-Wavelength Absorption Edge of C_{60} Films with Thicknesses of 5000 and ∼1000 nm

In this work, to study the energy structure of the long-wavelength edge of the output absorption spectra of C_{60} films with a thicknesses of 5000 and ∼1000 nm (Fig. 1, *a*, curves *1* and *2*, respectively), the method of approximating the corresponding spectral contours by a sum of Gaussian functions using the Origin software without baseline subtraction was used. Below, for convenience, the resulting composite contour and the individual Gaussian functions are labeled as the summary contour (total or cumulative) and Gaussian, respectively.

A complete fit of the output spectrum of a C_{60} film with a thickness of 5000 nm (Fig. 2, *b*, curve *1*) was obtained with an allowable standard deviation of $1 \times \times 10^{-9}$ (Chi-Square) and a coefficient of determination $R^2 = 0.9998$. The relative measurement errors in the abscissa E_m values of Gaussian maxima at 1.829 and 2.026 eV are 0.14 and 0.16%, respectively.

Fig. 2, *b* shows the full Gaussian contour of 1.829 eV (curve *3*) and the long-wavelength half of the Gaussian contour of 2.026 eV (curve *4*). The Gaussian E_m value of 2.026 eV is 0.027 eV larger than the energy of the singlet $A_g \to 1T_{1g}$ transition of the C_{60} film, equal to 1.999 eV. The contributions of the Gaussians at 1.829 and 2.026 eV to the output spectrum of the 5000 nm thick C_{60} film (Fig. 2, curves *3* and *4*) were estimated by their areas, which were 0.022 and 0.4925 a.u. (the full area and half the area of the Gaussians at 1.829 and 2.026 eV, respectively). The ratios of the areas of these Gaussians to the total area were 4% and 96%, i.e., the main contribution is made by the Gaussian at 2.026 eV.

At $E_0 = 1.414$ eV, the ordinates of the initial points D_0 of the summary spectrum and the

Gaussians at 1.829 and 2.026 eV coincide and are 2.807×10^{-5} a.u. (Fig. 2, *a*, curves *2*, *3* and *4*, respectively), whereas the ordinate of the output spectrum is $D_0 = 1.777 \times 10^{-3}$ a.u. (curve *1*) is approximately two orders of magnitude larger. A sharp increase and coincidence values of D of the output, summary spectra, and the Gaussian function of 2.026 eV are observed at E greater than 1.510 and 1.620 eV, respectively.

For the first time, a vibronic progression was described with estimated band maxima at 1.51 ($0 \to 0$ transition); 1.68; 1.83; 1.93 and 2.00 eV in the $\log D = f(E)$ spectrum of a C_{60} film with a thickness of ∼1000 nm, and the nature of this progression was not explained [9]. In order to clarify the nature of this progression, the long-wavelength edge of the $\log \alpha = f(E)$ spectrum of a C_{60} film with a thickness of 5000 nm was approximated by a sum of Gaussians with baseline subtraction. A progression with band maxima at 1.536 ($0 \to 0$ transition), 1.640, 1.757, 1.855 and 1.938 eV was obtained, and it was suggested that it is due to a triplet exciton [14–16]. The position of the 2.00 eV band is close to that of the 1.999 eV band assigned to the $A_g \to 1T_{1g}$ transition in the C_{60} film [3], i.e. it does not belong to the vibronic progression. Comparison of the two progressions shows that an additional band at 1.757 eV is observed in the 5000-nm-thick C_{60} film. Moreover, the vibronic bands at 1.536, 1.640, 1.855 and 1.938 eV are shifted by 0.026, (–0.040), 0.025 and 0.008 eV relative to those for the C_{60} film with a thickness of ∼1000 nm, respectively. These shifts are attributable to differences in the methods used to determine the positions of the band maxima. The average vibrational quantum energy of the vibronic progression of a C_{60} film with a thickness of 5000 nm is 0.1005 eV (811 cm^{-1}).

The Gaussian maximum at 1.829 eV nearly coincides with the 1.830 eV vibronic band of a ∼1000 nm thick C_{60} film and is red-shifted by 0.026 eV relative to the 1.855 eV vibronic band of a 5000 nm thick C_{60} film. The energies of the first long-wavelength electronic transitions of C_{60} and C_{70} are 1.999 and 1.889 eV [3]. Thus, in going from C_{60} to C_{70}, the size of the π-electron system increases, which causes a red shift of the first long-wavelength band by 0.110 eV. Since the Gaussian centered at 1.829 eV does not fall within the energy range of 1.889–1.999 eV, it cannot be associated with absorption by the C_{62} and C_{64} fullerenes [2], whose π systems are intermediate in size between those of C_{60} and C_{70}, and whose long-wavelength bands should lie within the photon energy range of 1.889–1.999 eV. In view of the above, it can be assumed that the Gaussian at 1.829 eV is the vibronic band of the C_{60} triplet exciton.

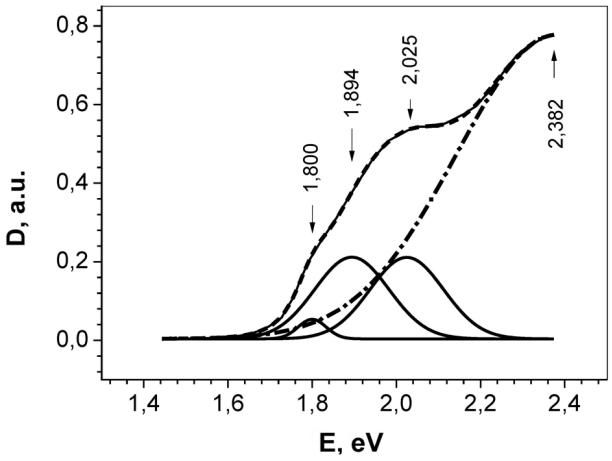

Fig. 3. Approximation of the long-wavelength edge of the absorption spectrum of a ∼1000 nm thick C_{60} film by a sum of Gaussian functions: thin solid line – output spectrum; dashed line – summary spectrum; solid thick lines – Gaussians 1.800, 1.894, 2.025 and dash-dotted line – Gaussian 2.382 eV

In Ref. [3], bands with energies of 2.022 and 2.176 eV were observed in the C_{70} film and 1.999 eV in the C_{60} film both with a thickness of 20 nm. In our work, these bands are represented by a single Gaussian centered at 2.026 eV (Fig. 2, *b*, curve *4*) due to their strong overlap. It can be assumed that the Gaussian function with a maximum at 2.026 eV is due to the combined absorption by molecules of the main component C_{60} and the C_{70} impurity.

The output absorption spectrum of a ∼1000 nm thick C_{60} film (Fig. 1, *a*, curve *2*) is approximated by a sum of Gaussian functions without baseline subtraction. A completed approximation was obtained with an acceptable standard deviation of 1×10^{-9} (Chi-square) and a coefficient of determination of $R^2 = 0.9999$. The full Gaussian contours at 1.800, 1.894 and 2.025 eV and the long-wavelength half of the Gaussian contour of 2.382 eV were obtained with relative errors in the corresponding E_m values of 0.15, 0.22 and 1.86, and 0.27%, respectively (Fig. 3).

The areas of Gaussians centered at 1.800, 1.894, 2.025, and 2.382 eV accounted for 1.3, 14.0, 13.9, and 70.8% of their total area, respectively. Thus, the

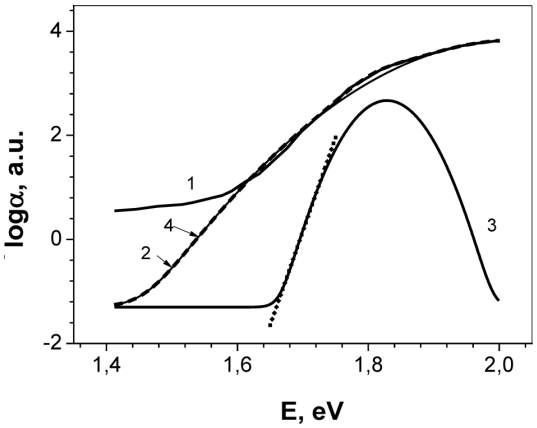

Fig. 4. Long-wavelength edge of the spectra $\log \alpha = f(E)$ of a C_{60} film with a thickness of 5000 nm: output spectrum (*1*); summary spectrum (dashed line, *2*); Gaussian at 1.829 eV (*3*) and long-wavelength half of the Gaussian at 2.026 eV (*4*). The dotted line indicates the extrapolated straight line section of curve *3*

Table 1. **Values of E_m and areas A under Gaussian curves of C_{60} films with thicknesses of 5000 and ∼1000 nm in different spectral regions**

d, nm	5000		∼1000			
E_m, eV	1.829	2.026	1.800	1.894	2.025	2.382
Relative error, %	0.14	0.22	0.15	2.24	1.86	0.27
Area A, a.u.	0.022	0.985	0.004	0.046	0.045	0.464
Relative error, %	21.7	3.24	29.3	5.78	6.89	5.86
Spectral region, eV	1.414–1.998		1.448–2.371			

largest contributions to the absorption of the output spectrum (Fig. 3, thin solid line) are made by the Gaussians at 1.894, 2.025 and 2.382 eV.

The abscissas *Em* of the Gaussians centered at 2.025 and 2.382 eV are 0.026 eV higher and 0.087 eV lower than the energies of the $A_g \to 1T_{1g}$ and $A_g \to$ $\to 1T_{1u}$ transitions of C_{60} films at 1.999 and 2.469 eV, respectively. Moreover, the abscissa of the maximum of the Gaussian at 2.382 eV is close in magnitude to the transition energy $e_2'' \to e_1''$ of C_{70} films, reported as 2.344 eV in [3]. This means that the Gaussians at 2.025 and 2.382 eV are due to the combined absorption of C_{60} and C_{70} molecules. The Gaussian maximum at 1.894 eV is close to the absorption band at 1.889 eV of C_{70} films ($a_2'' \to a_1''$ transition) [3], i.e., it is due to the absorption of C_{70} molecules. This shows that the ∼1000 nm thick C_{60} film contains more C_{70} impurity than the 5000 nm-thick C_{60} film, in the absorption spectrum of which this Gaussian is absent.

The Gaussian maximum at 1.800 eV is close to the position of the 1.83 eV band of a ∼1000 nm thick C_{60} film, therefore, it may correspond to the second vibronic band of the triplet exciton at 1.51 eV ($0 \to 0$ transition).

The E_m values and the areas A under the Gaussian contours (Figs 2*b* and 3) are given in Table 1. The comparison shows that the E_m values of Gaussian maxima were determined using Origin with a relative measurement error ranging from 0.14 to 2.24%. The Gaussian maxima at 1.829, 2.026, 1.800 and 2.382 eV are approximated with the highest accuracy (the relative errors of 0.14–0.27%). The relative measurement error of the Gaussian maxima at 1.894 and 2.025 eV exceed 1%, amounting to 2.24 and 1.86%, respectively. The values of the integral intensities of Gaussians can be estimated from their areas A. The areas of the Gaussians centered at 1.829 and 1.800 eV were determined with relative errors of 21.7 and 29.3%, respectively. For the remaining Gaussians, this error does not exceed 6.89%.

The data presented in Table 1 for C_{60} films with a thickness of 5000 and ∼1000 nm show that the energy structure of the long-wavelength edge of their spectra is formed by several electronic transitions. The values of Eu and E_g for these transitions are of scientific interest and can be determined using Eqs (2) and (4), respectively.

6. Determination of E_u and E_g Values for a 5000 nm Thick C_{60} Film in the Long-Wavelength Edge Region

The $\log \alpha = f(E)$ spectrum of a 5000 nm thick C_{60} film (Fig. 4) was obtained by calculating the decimal logarithm of the ordinate of the $\alpha = f(E)$ spectrum (Fig. 1, *b*, curve *1*).

The contours of the summary spectrum and the Gaussian centered at 2.026 eV coincide in the region of 1.414–1.998 eV (Fig. 4, curves *2* and *4*, respectively). In the region of 1.414–1.619 eV, the contour of the output spectrum lies above that of the summary spectrum (curves *1* and *2*, respectively). The summary spectrum (curve *2*) lies above the output spectrum (curve *1*) in the regions of 1.619–1.698 eV and 1.747–1.864 eV. The contours of these spectra coincide in the region of 1.864–1.998 eV. The main

Table 2. **Coordinates E_0 and D_0 of the initial point of the spectrum $D(E)$, photon energies E_1 and E_2 at the beginning and end of the straightline section, coefficient k_u, its error $\Delta k_u/k_u$, and Urbach energy E_u for all $\log\alpha(E)$ spectra of the C_{60} film with a thickness of 5000 nm**

No.	E_0, eV	$D_0 \times 10^3$ a.u.	E_1, eV	E_2, eV	k_u, eV^{-1}	$\Delta k_u/k_u$, %	E_u, meV	Contour
1	***1.414***	***1.777***	***1.633***	***1.770***	***11.6394***	***2.28***	***37.31***	***Output***
2	1.414	1.777	1.633	1.696	12.4839	4.21	34.79	Output 1
3	1.414	1.777	1.696	1.770	11.3237	2.83	38.34	Output 2
4	***1.414***	***0.028***	***1.451***	***1.789***	***12.7119***	***0.29***	***34.16***	***Summary***
5	1.414	0.028	1.451	1.625	14.5082	0.09	29.93	Summary (1)
6	1.414	0.028	1.625	1.789	10.8108	0.12	40.17	Summary (2)
7	1.414	0.025	1.667	1.726	35.7342	0.39	12.15	Gaussian 1.829 eV
8	***1.414***	***0.028***	***1.442***	***1.737***	***12.2899***	***0.39***	***35.34***	***Gaussian 2.026 eV***
9	1.414	0.028	1.442	1.636	14.3588	0.12	30.25	Gaussian 2.026 eV (1)
10	1.414	0.028	1.636	1.737	9.1062	0.44	47.69	Gaussian 2.026 eV (2)

contribution to the output spectrum is made by the long-wavelength edge of the Gaussian at 2.026 eV (curve *4*). The contribution of the 1.829 eV Gaussian (curve *3*) to the output spectrum is observed in the region of 1.640–1.998 eV. The steepness of the long-wavelength edge of the Gaussian at 1.829 eV is larger than that of the 2.026 eV Gaussian (curves *3* and *4*, respectively).

In our work, the long-wavelength halves of all spectral contours were approximated by straight lines using the Origin software. For example, this line is shown in Fig. 4 only for the Gaussian dependence centered at 1.829 eV (dashed line to curve *3*). For other curves, approximate straight lines are omitted so as not to complicate Fig. 4. Two linear sections were observed for the contours of the output and summary spectra, as well as for the Gaussian curve at 2.026 eV. The end of the first (long-wavelength) section coincides with the beginning of the second (short-wavelength) section. The E_u value was determined for three sections: longwave, shortwave, and all section together (combined). The E_u value was determined for three sections: longwave, shortwave, and all section together (combined).

The combined region includes all contour points between the beginning of the long-wavelength region and the end of the short-wavelength region. The obtained data are given in Table 2. The data for the combined regions of the output and summary spectra and the Gaussian centered at 2.026 eV are shown in bold italics.

In the combined spectral region of the output spectrum contour, the obtained k_u value is 11.6394 eV^{-1} with a relative error of 2.28%, and the value of E_u determined using Eq. (2) is 37.31 meV with the same error (Table 2, cells (1, 6), (1, 7) and (1, 8) respectively, where the first and second numbers correspond to the row and column, respectively). This value of E_u is close to the value of 37.00 meV reported in [12]. In the long-wavelength and short-wavelength regions, the k_u values are 12.4839 and 11.3267 eV^{-1} with errors of 4.21 and 2.38% (cells (2, 6) and (3, 6)), and the E_u value are 34.79 and 38.34 meV (cells (2, 8) and (3, 8)), respectively. The average E_u value for these regions of 36.57 meV is close to the value for the combined region of 37.31 meV (cell (1, 8)). The coordinates of the initial point of the output spectrum E_0 and D_0 are 1.414 eV and 1.777×10^{-3} a.u. (cells (1, 2) and (1, 3), respectively).

In the combined region, the value $k_u = 12.7119$ eV^{-1} is obtained for the contour of the summary spectrum with an error of 0.29%, and E_u is 34.16 meV (cells (4, 6), (4, 7), and (4, 8) respectively). Compared with the output spectrum, the k_u value is larger with a much smaller error, and the E_u value is lower (cells (1, 6), (1, 7), and (1, 8) respectively). The D_0 value of the summary spectrum is 2.8×10^{-5} a.u. (cell (4, 3)) and is approximately two orders of magnitude smaller than that of the output spectrum (cell (1, 3)). In the long-wavelength and short-wavelength regions of the summary spectrum contour, the k_u values are 14.5082 and 10.8108 eV^{-1} with errors of 0.09 and 0.12%, and the E_u values are 29.93 and 40.17 meV, respectively (cells (5, 6) and (6, 6), (5, 7) and (6, 7), (5, 8) and (6, 8) respectively). The average E_u value for these regions of

Table 3. **Values of the photon energies E_1 and E_2 at the beginning and end of the linear section, the coefficient k_g and its error $\Delta k_g/k_g$, the optical band gap energy E_g, and Urbach energy E_u for all spectra of the Tauc function $(\alpha^* E)^{0.5} = f(E)$ of a 5000 nm thick C_{60} film**

No.	E_1, eV	E_2, eV	k_g, $\mathrm{cm}^{-0.5} \cdot \mathrm{eV}^{0.5}$	$\Delta k_g/k_g$, %	E_g, eV	E_u, meV	Contour
1	***1.722***	***1.939***	***374.44274***	***1.81***	***1.670***	***37.31***	***Output***
2	1.746	1.822	425.13565	3.35	1.683	34.79	Output (1)
3	1.822	1.939	347.32178	2.43	1.653	38.34	Output (2)
4	***1.730***	***1.932***	***377.78141***	***0.29***	***1.670***	***34.16***	***Summary***
5	1.745	1.838	427.10408	0.24	1.684	29.93	Summary (1)
6	1.838	1.932	427.10408	0.24	1.670	40.17	Summary (2)
7	1.742	1.802	307.18546	0.47	1.718	12.15	Gaussian 1.829 eV
8	***1.727***	***1.952***	***389.85058***	***0.29***	***1.686***	***35.34***	***Gaussian 2.026 eV***
9	1.727	1.826	327.96487	0.55	1.669	30.25	Gaussian 2.026 eV (1)
10	1.826	1.952	396.29183	0.35	1.687	47.69	Gaussian 2,026 eV (2)

35.05 meV is close to that of 34.16 meV (cell (4, 8)) for the combined region.

For the Gaussian centered at 1.828 eV in the region of 1.667–1.726 eV, the k_u value is 35.7342 eV^{-1} with an error of 0.39%, and the E_u value is 12.15 meV (cells (7, 6), (7, 7) and (7, 8) respectively). The k_u value is significantly higher, whereas the E_u value is significantly lower, than the corresponding values for the output and summary spectra. The value of D_0 is 2.5×10^{-5} a.u. (cell (7, 3)).

For the Gaussian centered at 2.026 eV in the combined region, k_u, and E_u are 12.2899 eV^{-1} and 35.34 meV, respectively (cells (8, 6) and (8, 8)). They are close to those for the summary spectrum (cells (4, 6) and (4, 8) respectively). In the long- and short-wavelength regions for the Gaussian at 2.026 eV, the k_u values and E_u are 14.3588 and 9.1062 eV^{-1} with errors of 0.12 and 0.44%, 30.25 and 47.69 meV (cells (9, 6) and (10, 6), (9, 7) and (10, 7), (9, 8) and (10, 8) respectively). These values are close to the corresponding values for the long- and short-waves regions of the summary spectrum (rows 5 and 6, columns 6–8, respectively). The average E_u value for these regions, 38.97 meV, is larger than that for the combined region, 35.34 meV.

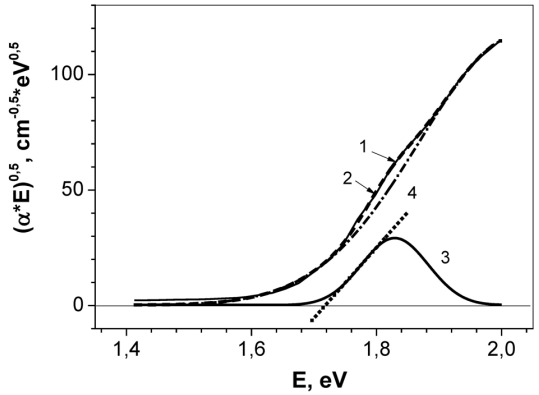

Fig. 5. Spectral dependences of the Tauc function $(\alpha^* E)^{0.5} = f(E)$ for a C_{60} film with a thickness of 5000 nm. All notations are the same as in Fig. 4

The spectral dependences of the Tauc function $(\alpha^* E)^{0.5} = f(E)$ and the corresponding values of E_1, E_2, k_g, $\Delta k_g/k_g$, E_g and E_u obtained on their basis are shown in Fig. 5 and Table 3, respectively. Fig. 5 shows an approximating straight line of the linear section (dashed line) for curve *3* only. For other curves, these lines are not shown so as not to complicate Fig. 5. The value of E_g for all contours of the 5000 nm thick C_{60} film was obtained by two methods: by calculation using Eq. (4) for the points on the linear sections of the graph and by extrapolating the straight lines of these sections to zero of the Tauc function $y = (\alpha^* E)^{0.5}$. In both cases, the obtained E_g values were in close agreement. For convenience, only one E_g value is given below. The relative error of E_g was equal to the error of the coefficient k_g. The E_g values for the contours of the output and summary spectra and for the Gaussian centered at 2.026 eV are highlighted in bold italics.

For the contour of the output spectrum in the combined, long-wavelength and short-wavelength regions, the values of E_g were 1.670, 1.683, and 1.653 eV (Table 3, cells (1, 6), (2, 6) and (3, 6), respectively). The E_g value of 1.670 eV is close to the average E_g value of 1.668 eV for the long- and short-wavel regions.

In the combined, long-wavelength and short-wavelength regions of the summary spectrum contour, the E_g values are 1.670, 1.684, and 1.670 eV, respectively (Table 3, cells (4, 6), (5, 6) and (6, 6)). Notably, the E_g values for the combined and short-wavelength regions are identical.

For the Gaussian contour centered at 1.829 eV, the obtained E_g value is 1.718 eV (cell (7, 6)). This value is the largest among those obtained for all the contours.

The E_g values for the Gaussian contour centered at 2.026 eV are 1.686, 1.669, and 1.687 eV, respectively, (cells (8, 6), (9, 6) and (10, 6); notably, the values for the combined and short-wavelength regions are close. All E_g values (column 6) given in Table 3 correspond to the previously determined E_u values (column 7), which are given in Table 2 (column 8).

Analysis of the data for E_g and E_u presented in Table 3 (columns 6 and 7, respectively) showed that for all contours of the 5000 nm thick C_{60} film, a larger E_u value corresponds to a smaller or equal E_g value. The difference $\Delta E_u/E_u$ between the largest and smallest E_u values relative to the largest value is 9.26, 25.42 and 36.56%, and the same relative difference $\Delta E_g/E_g$ is 1.78, 0.83 and 1.07% for the contours of the output and summary spectra and the Gaussian centered at 2.026 eV, respectively. Therefore, the discrepancy between the E_g values obtained using Origin program for individual contours is much smaller than that for E_u.

The $D_0 \times 10^3$, E_u and Eg values of the output spectrum of a 5000 nm thick C60 film are 1.777 a.u., 37.31 meV and 1.670 eV (Tables 2 and 3, row 1), whereas the corresponding values for the summary spectrum are 0.028 a.u., 34.16 meV and 1.670 eV (Tables 2 and 3, row 4). The ratio of the $D_0 \times 10^3$ values of these spectra is $1.777/0.028 \approx 63.5$. When the $D_0 \times 10^3$ values of the output spectrum of this film increases from 1.777 to 3.547 a.u., the values of E_u and E_g are 37.76 meV and 1.675 eV. In this case, the values of $D_0 \times 10^3$, E_u and E_g of the summary spectrum are 1.800 a.u., 41.12 meV and 1.669 eV, and the ratio of the $D_0 \times 10^3$ values of the output and summary spectra is decreases to $3.547/1.800 \approx 1.97$. With a further increase in the $D_0 \times 10^3$ value of the output spectrum to 5.327 a.u., E_u and E_g are 39.26 meV and 1.675 eV. In this case, the values of $D_0 \times 10^3$, E_u and E_g of the summary spectrum are 3.578 a.u., 42.48 meV and 1.670 eV, and the ratio of the $D_0 \times 10^3$ values of the output and summary spectra is decreases further to $5.327/3.578 \approx 1.49$. Therefore, with an increase in the value of $D_0 \times 10^3$ of the initial spectrum within the range of 1.777–5.327 a.u., the values of E_u and E_g change only slightly. Moreover, the ratio of the $D_0 \times 10^3$ values of the output and summary spectra decreases from 63.5 to 1.49.

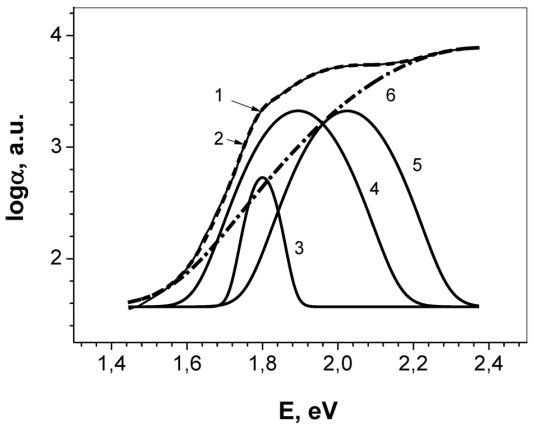

Fig. 6. Long-wavelength edge of the $\log \alpha = f(E)$ spectra of the C_{60} film with a thickness of ∼1000 nm: *1* – output spectrum (thin solid line); *2* – summary spectrum (dashed line); *3*, *4* and *5* – Gaussians centered at 1.800, 1.894 and 2.025 eV; *6* – long-wavelength half of the Gaussian centered at 2.382 eV, respectively

7. Determination of the E_u and E_g Values of Electronic Transitions at the Long-Wavelength Edge of a C_{60} Film with a Thickness of ∼1000 nm

The output spectrum $\log \alpha(E)$ of a C_{60} film with a thickness of ∼1000 nm (Fig. 6) was obtained by taking the decimal logarithm of the ordinate of the spectrum $\alpha = f(E)$ (Fig. 1, *b*, curve *2*) and approximating it by a sum of Gaussians. Gaussians centered at 1.800, 1.894, 2.025 and 2.382 eV were obtained.

The contours of the output and summary spectra nearly coincide (Fig. 6, curves *1* and *2*, respectively). The results obtained are given in Table 4. The data for the combined regions of the output and summary spectra are shown in bold italics. The E_u value of 57.36 meV for the output spectrum contour (cell (1, 8)) is smaller than the value of 61 meV reported in Ref. [9]. The E_u value of 57.36 meV is 1.537 times larger than that for the 5000 nm thick C_{60} film

Table 4. **Coordinates E_0 and $D_0 \times 10^3$ of the initial point of the spectrum $D(E)$, photon energies E_1 and E_2 of the beginning and end of the straight section, coefficient k_u, its errors $\Delta k_u/k_u$, Urbach energy E_u for all spectra $\log \alpha(E)$ of the C_{60} film with a thickness of ∼1000 nm**

No.	E_0, eV	$D_0 \times 10^3$ a.u.	E_1, eV	E_2, eV	k_u, eV^{-1}	$\Delta k_u/k_u$, %	E_u, meV	Contour
1	***1.448***	***3.550***	***1.611***	***1.794***	***7.5709***	***2.42***	***57.36***	***Output***
2	1.448	3.550	1.611	1.728	6.8999	1.56	62.94	Output 1
3	1.448	3.550	1.728	1.794	8.2005	7.59	52.96	Output 2
4	***1.448***	***4.100***	***1.637***	***1.790***	***8.2129***	***0.37***	***52.88***	***Summary***
5	1.448	4.100	1.637	1.720	7.6512	0.40	56.76	Summary 1
6	1.448	4.100	1.720	1.790	8.3946	0.65	51.74	Summary 2
7	1.448	3.707	1.708	1.758	15.4911	0.83	28.04	Gaussian 1.800 eV
8	1.448	3.707	1.644	1.761	8.5436	0.22	50.93	Gaussian 1.894 eV
9	1.448	3.707	1.776	1.896	8.6383	0.22	50.28	Gaussian 2.025 eV
10	1.448	4.093	1.636	1.901	4.0051	0.09	108.44	Gaussian 2.382 eV

Table 5. **Values of the photon energies E_1 and E_2 at the beginning and end of the linear section, the coefficient k_g, its error $\Delta k_g/k_g$, the optical band gap energy E_g and the Urbach energy E_u for all spectra of the Tauc function $(\alpha^* E)^{0.5} = f(E)$ of a C_{60} film with a thickness of ∼1000 nm**

No.	E_1, eV	E_2, eV	k_g, cm$^{-0,5}\cdot$ eV^{0,5}	$\Delta k_g/k_g$, %	E_g, eV	E_u, meV	Contour
1	***1.661***	***1.893***	***285.86578***	***5.71***	***1.598***	***57.36***	***Output***
2	1.725	1.793	438.21003	3.29	1.655	62.94	Output 1
3	1.793	1.944	226.27075	2.07	1.524	52.96	Output 2
4	***1.649***	***1.894***	***285.44894***	***1.02***	***1.596***	***52.88***	***Summary***
5	1.724	1.800	427.03104	0.44	1.652	56.76	Summary 1
6	1.800	1.944	287.62332	0.29	1.524	51.74	Summary 2
7	1.728	1.781	324.31559	0.81	1.692	28.04	Gaussian 1.800 eV
8	1.707	1.838	279.13911	0.41	1.634	50.93	Gaussian 1.894 eV
9	1.843	1.966	296.79682	0.27	1.769	50.28	Gaussian 2.025 eV
10	1.876	2.234	224.85533	0.23	1.699	108.44	Gaussian 2.382 eV

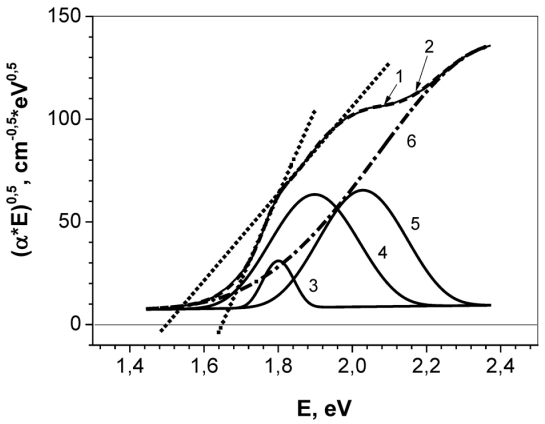

Fig. 7. Spectral dependences of the Tauc function $(\alpha^* E)^{0.5} = f(E)$ for a C_{60} film with a thickness of ∼1000 nm. All notations are the same as in Fig. 6. The dashed lines indicate the extrapolated straight-line sections of curve *1*

(37.31 meV), which may indicate a lower degree of structural ordering in the ∼1000 nm thick C_{60} film.

For the contour of the summary spectrum, the obtained E_u value is 52.88 meV (Table 4, cell (4, 8)), which is smaller than that for the contour of the output spectrum (57.36 meV). The smallest and largest E_u values of 28.04 and 108.44 meV were obtained for the Gaussians centered at 1.800 and 2.382 eV, respectively.

The spectral dependences of the Tauc function $(\alpha^* E)^{0.5} = f(E)$ and the values of E_1, E_2, k_g, $\Delta k_g/k_g$, E_g and E_u obtained on their basis are shown in Fig. 7 and Table 5, respectively. In Fig. 7, the approximating straight lines for the two linear sections (dashed lines) are shown only for curve *1*. For other curves, these lines are omitted to avoid cluttering Fig. 7. The E_g value for the combined contour regions

of the output and summary spectra is highlighted in bold italics. All E_g values (column 6) given in Table 5 correspond to the previously determined E_u values (column 7) given in Table 4 (column 8). The largest E_g value of 1.769 eV was obtained for the Gaussian centered at 2.025 eV.

The values of $D_0 \times 10^3$, E_u and E_g of the output spectrum of the C_{60} film with a thickness of ∼1000 nm are 3.550 a.u., 57.36 meV and 1.598 eV (Tables 4 and 5, row 1), whereas the corresponding values for the summary spectrum are 4.100 a.u., 52.88 meV, and 1.596 eV (Tables 4 and 5, row 4). The ratio of the $D_0 \times 10^3$ values for these spectra is $3.550/4.100 \approx 0.87$. Thus, the initial ordinate $D_0 \times \times 10^3 = 3.550$ a.u. of the output spectrum is optimal for determining the E_u and E_g values of C_{60} films with thicknesses of 5000 and ∼1000 nm.

Therefore, the above results indicate that C_{60} films with thicknesses of 5000 and ∼1000 nm contain C_{70} impurity molecules. C_{70} molecules are formed during the synthesis of C_{60} and are not completely removed by crystallization from solution and column chromatography. During the thermal deposition of the starting C_{60} powder onto solid substrates, the amount of C_{70} may increase under the influence of temperature. Electronic transitions associated with C_{70} affect the energy structure of the long-wavelength absorption edge of C_{60} films. A detailed study of purity of these films remains relevant, because the purity of C_{60} films significantly affects the efficiency of solar cells and other devices based on C_{60}-containing composites. This indicates the need to continue such research.

8. Conclusions

The energy structure of the long-wavelength edge of the absorption spectra of C_{60} films with thicknesses of 5000 and ∼1000 nm in the region of 1.414–1.998 eV and 1.448–2.371 eV, respectively, was studied in detail. It was found that in C_{60} films with a thickness of 5000 nm, this structure is formed by the sum of Gaussians 1.829 and 2.026 eV and in C_{60} films with a thickness of ∼1000 nm, it is formed by the sum of Gaussians centered at 1.800, 1.894, 2.025 and 2.382 eV.

The main contribution to the long-wavelength absorption edge of C_{60} films with a thickness of 5000 nm is made by the Gaussian at 2.026 eV, and that of C_{60} films with a thickness of ∼1000 nm – by the Gaussians at 1.894, 2.025, and 2.382 eV.

For C_{60} films with thicknesses of 5000 and ∼1000 nm, the Gaussians at 1.829, and 1.800 eV, respectively, may correspond to vibronic bands of the triplet exciton, whereas, the Gaussians centered at 2.026 and 2.025 eV are due to the combined absorption of C_{60} and C_{70} molecules, respectively. In C_{60} films with a thickness of ∼1000 nm, the Gaussian at 1.894 is attributed to absorption by C_{70} molecules, and the Gaussian of 2.382 eV is due to the co-absorption of C_{60} and C_{70} molecules.

The E_u value for the output spectra of C_{60} films with a thickness of 5000 and ∼1000 nm is 37.31 and 57.36 meV, and E_g is 1.670 and 1.598 eV, respectively. A smaller value of E_u indicates a greater ordering of the 5000 nm thick C_{60} films.

Two straight-line sections were observed at the long-wavelength edge of the curves of $\log \alpha = f(E)$ and $(\alpha \times E)^{0.5} = f(E)$ of the output and summary spectra of C_{60} films with thicknesses of 5000 and ∼1000 nm. The average values of E_u and E_g for these regions are close to those for the output spectra of these films. The largest and smallest E_u values of 108.40 and 12.15 meV were obtained for Gaussians centered at 2.382 and 1.829 eV in C_{60} films with thicknesses of ∼1000 and 5000 nm, respectively.

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1. H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl, R.E. Smalley. C_{60}: Buckminsterfullerene. *Nature* **318** (6042), 162 (1985).
2. H. Ajie, M.M. Alvarez, S.J. Anz, R.D. Beck, F. Diederich, K. Fostiropoulos, D.R. Krätschmer, M. Rubin, K.E. Schriver, D. Sensharma, R.L. Whetten. Characterization of the soluble all-carbon molecules C_{60} and C_{70}. *J. Phys. Chem.* **94**, 8630 (1990).
3. M.P. Gorishnyi. Surface morphology of the films of the C_{60}/C_{70} fullerene mixture. Identification of C_{60} and C_{70} in the C_{60}/C_{70} films using absorption spectra. *Ukr. J. Phys.* **68** (5), 318 (2023).
4. Y. Yi, V. Coropceanu, J.-L. Bredas. Exciton-dissociation and charge-recombination processes in pentacene/C_{60} solar cells: Theoretical insight into the impact of interface geometry. *J. Am. Chem. Soc.* **131** (43), 15777 (2009).
5. P. Brown, P.V. Kamat. Quantum dot solar cells. Electrophoretic deposition of CdSe–C_{60} composite films and capture of photogenerated electrons with nC_{60} cluster shell. *J. Am. Chem. Soc.* **130** (28), 8890 (2008).
6. H. Yi, D. Huang, L. Qin, G. Zeng, C. Lai, M. Cheng, S. Ye, B. Song, X. Ren, X. Guo. Selective prepared carbon nanomaterials for advanced photocatalytic application in envi-

ronmental pollutant treatment and hydrogen production. *Appl. Catal. B* **239**, 408 (2018).
7. P. Mroz, G.P. Tegos, H. Gali, T. Wharton, T. Sarna, M.R. Hamblin. Photodynamic therapy with fullerenes. *Photoch. Photobid. Sci.* **6** (11), 1139 (2007).
8. S. Afreen, K. Muthoosamy, S. Manickam, U. Hashim. Functionalized fullerene (C_{60}) as a potential nanomediator in the fabrication of highly sensitive biosensors. *Biosens. Bioelectron.* **63**, 354 (2015).
9. A. Scumanich. Optical absorption spectra of carbon 60 thin films from 0.4 to 6.2 eV. *Chem. Phys. Lett.* **182** (5), 486 (1991).
10. A. Scumanich. Optical spectra of fullerenes: C_{60} a new amorphous semiconductor? *Mat. Res. Soc. Symp. Proc.* **270**, 299 (1992). Material Research Society.
11. V.K. Dolganov, O.V. Zharikov, I.N. Kremenskaja, K.P. Meletov, Yu.A. Ossipyan. High pressure study of the absorption edge of crystalline C_{60}/C_{70} mixture. *Solid State Commun.* **83** (1), 63 (1992).
12. T. Gotoh, S. Nonomura, H. Watanabe, S. Nitta, D. Han. Temperature dependence of the optical-absorption edge in C_{60} thin films. *Phys. Rev. B* **58** (15), 10060 (1998).
13. E.Yu. Kolyadina, L.A. Matveeva, P.L. Neluba, E.F. Venger. Analysis of the fundamental absorption edge of the films obtained from the C_{60} fullerene molecular beam in vacuum and effect of internal mechanical stresses on it. *Semiconductor Physics, Quantum Electronics & Optoelectronics* **18** (3), 349 (2015).
14. M.P. Gorishnyi. Determination of the Urbach energy E_u and the optical band gap E_g of submicron C_{60} and C_{70} fullerene films. *Fizyka Nyzkykh Temperatur/Low Temperature Physics* **51** (2), 192 (2025).
15. M.P. Gorishnyi. Determination of the Urbach energy $E_u$and the optical band gap E_g of submicron C_{60} and C_{70} fullerene films. *Low Temp. Phys.* **51**, 174 (2025).
16. M.P. Gorishnyi. Determination of the Urbach energy E_u and the optical band gap E_g in submicron C_{60} and C_{70} fullerene films. Dependences of E_u and E_g of the films on their thickness in the range 20–5000 nm. *Ukr. J. Phys.* **70** (5), 303 (2025).
17. S. Pfuetzner, J. Meiss, A. Petrich, M. Riede, K. Leo. Improved bulk heterojunction organic solar cells employing C_{70} fullerenes. *Appl. Phys. Lett.* **94** (22), 223307 (2009).
18. J. Klein, L. Kampermann, B. Mockenhaupt, M. Behrens, J. Strunk, G. Bacher. Limitations of the Tauc Plot Method. *Adv. Funct. Mater.* **33**, 2304523 (2023).
19. J. Tauc, R. Grigorovici, A. Vancu. Optical properties and electronic structure of amorphous Germanium. *Phys. Stat. Sol.* **15**, 627 (1966).

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АПРОКСИМАЦІЯ ДОВГОХВИЛЬОВОГО КРАЮ СПЕКТРІВ ПОГЛИНАННЯ СУМОЮ ФУНКЦІЙ ГАУСА І ВИЗНАЧЕННЯ ВЕЛИЧИН ЕНЕРГІЇ УРБАХА E_u ТА ОПТИЧНОЇ ШИРИНИ ЗАБОРОНЕНОЇ ЗОНИ E_g ПЛІВОК C_{60} ТОВЩИНОЮ 5000 І ∼1000 нм

Довгохвильовий край спектрів поглинання плівок C_{60} товщиною 5000 і ∼1000 нм апроксимовано сумою функцій Гауса (гаусіанів) в області 1,414–1,998 еВ і 1,448–2,371 еВ, відповідно. У плівках C_{60} товщиною 5000 нм цей край формується сумою гаусіанів 1,829 і 2,026 еВ, а в плівках C_{60} товщиною ∼1000 нм – сумою гаусіанів 1,800; 1,894; 2,025 і 2,382 еВ. Основний внесок у поглинання плівок C_{60} товщиною 5000 нм дає гаусіан 2,026 еВ, а в плівках C_{60} товщиною ∼1000 нм – гаусіани 1,894; 2,025 і 2,382 еВ. Величини E_u змінюються в межах 12,15–47,69 меВ і 28,04–108,44 меВ, а E_g – в межах 1,653–1,718 еВ і 1,524–1,769 еВ для плівок C_{60} товщиною 5000 і ∼1000 нм, відповідно.

Ключові слова: плівка, спектр поглинання, фулерени C_{60} і C_{70}, апроксимація, функція Гауса, гаусіан.