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Synthesis and Polar and Electrooptical Properties of a Butylamine Derivative of Fullerene C_{60}

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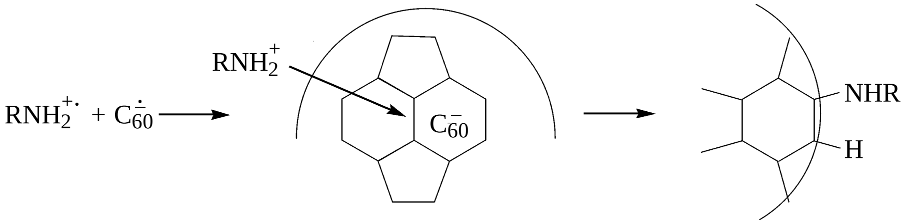
Abstract—A butylamine derivative of fullerene was prepared by the reaction of butylamine with fullerene C_{60}.The experimental electrooptical and dipole characteristics of the derivative were compared with the corresponding calculated PM3 data. The reaction product proved to be inhomogeneous in the number of the amine molecules added; it contains polar multiadducts of C_{60} with noncentrosymmetric distribution of covalently bound amino groups over the fullerene core.

The molecular characteristics and synthesis methods for fullerene derivatives attract much attention of materials scientists, as usually only chemical modification allows practical application of the unique properties of the framework forms of molecular carbon [1]. By contrast to fullerenes C_{60} and C_{70}, their amino derivatives are well soluble in organic solvents [2] and surpass unmodified fullerenes in photophysical properties [3]. A large potential of fullerene-containing materials and easy preparation of fullerene compounds with amines stimulated in recent years synthesis of various amine derivatives of C_{60} and C_{70} [2–5], including water-soluble derivatives suitable for studying the biological activity [6]. It was noted that the reaction products of fullerenes with amines include regioisomers with different numbers of amine molecules added [2, 7–10] and also that the composition and properties of amine derivatives of fullerenes are strongly dependent on the synthesis conditions [7].

The mechanism of covalent addition of primary amines to fullerenes C_{60} and C_{70} was studied by various spectral methods [2, 4, 8–10]. These studies showed that the reactions go in two steps, namely, one-electron transfer from the electron donor (amine) to electron acceptor (fullerene), yielding a radical anion $C_{60}^{\dot{-}}(C_{70}^{\dot{-}})$ and a radical cation $RNH_2^{+\cdot}$, which further recombine in the second step by the following scheme:



In this study, the reaction product (A–C_{60}) of butylamine (A) with fullerene C_{60} (C_{60}) was examined by the methods of dielectric polarization of molecules [11] and electrooptical Kerr effect [12] in toluene.

As already mentioned, reactions of primary amines with fullerenes, depending on the conditions, yield virtually inseparable multiadducts with difficult-to-control number of the amine molecules added. Therefore, estimation of the average number of the amine molecules added to fullerenes is always troublesome [2]. We took this into account when choosing the experimental methods in this study.

Importantly, studies of the regioselectivity of the addition to C_{60} [13] showed that energetically allowed are reactions between the reagent and the most reactive carbon atoms (C–C bonds between two hexa-

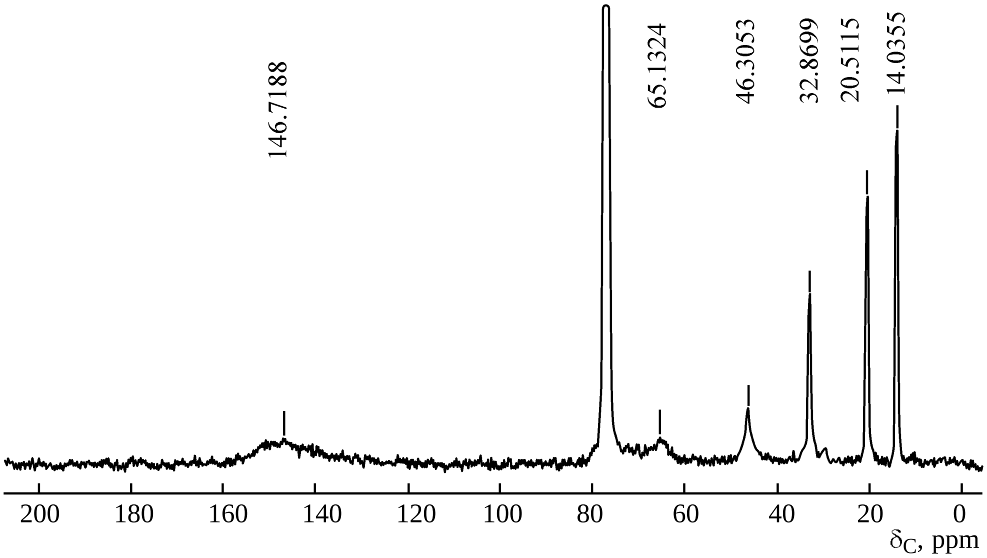


Fig. 1. ^{13}C NMR spectrum of the A–C_{60} sample in $CDCl_3$.

gons in the pyracyllene rings of C_{60}) of the hemisphere of the fullerene that already has been the site of one covalent addition. This means that reactions of fullerenes with primary amines can yield derivatives with noncentrosymmetric distribution of amines over the carbon core. Such derivatives of fullerene should exhibit significant polarity (owing to the C–N bond), which can easily be revealed by estimating their dipole moments μ or by studying their electrooptical properties in solutions.

The experimental dipole and electrooptical characteristics of the amine derivative of C_{60}, synthesized in this work, were compared with the corresponding calculated (PM3) data for the A–C_{60} molecules with 1–6 amine molecules added [14]. This allowed certain conclusions about the composition of the amine adducts. No additional approximations, except for the NDDO (neglect of diatomic differential overlap) approximation underlying the PM3 method, and no symmetry restrictions for the A–C_{60} molecule were taken in the calculations. Covalent bonding in the A–C_{60} synthesized was confirmed by the UV, ^{13}C NMR, and IR studies. The UV spectrum of A–C_{60} in chloroform is a monotonically descending curve with a small inflection near 260 nm, characteristic of covalent derivatives of C_{60} [6].

The ^{13}C NMR spectrum of A–C_{60} (Fig. 1) exhibits a broad maximum at 140–150 ppm, where the initial fullerene C_{60} has a narrow peak at 143 ppm, and monoadducts of the fullerene, a set of well-resolved lines. This suggests the presence of adducts with different numbers of incorporated amine molecules. The signals at 67–72 ppm, characteristic of sp^3 atoms of the modified fullerene, appear upon addition of amines at double bonds of fullerene [15, 16]. The signals at 14, 20, 33, and 46 ppm are attributed to the carbon atoms of the CH_3 and CH_2 groups in the butyl radical of A–C_{60}.

The IR spectrum of A–C_{60} (Fig. 2) contains no characteristic absorption bands of fullerene (527, 576, 1182, and 1428 cm^{-1}). The appearance of intense bands at 1000–1200 cm^{-1} (vibrations of the C–N bond) and disappearance of the absorption band of antisymmetric vibrations of the NH_2 groups at 3336 cm^{-1} confirm the covalent addition of A to C_{60} [5, 16].

The solutions of A–C_{60} in toluene exhibit positive electooptical Kerr effect. The equilibrium electrooptical properties of the substance under study were characterized by the specific Kerr constant K, which was determined by relationship (1):

$$K = \lim_{\substack{E\to 0\\ c\to 0}} [(\Delta n_c - \Delta n_0)/E^2 c]. \qquad (1)$$

Here, $\Delta n_c - \Delta n_0$ is the difference between the birefringences induced by the field in a solution of the substance under study at the concentration c and in the solvent, respectively, and E, electric field intensity.

The plots of the birefringence Δn vs. the squared electric field intensity E^2 for the A–C_{60} solutions were linear (Fig. 3a), which evidences molecular dispersity of the solutions. According to relationship (1), the slopes of the straight lines $\Delta n = f(E^2)$ give the Kerr

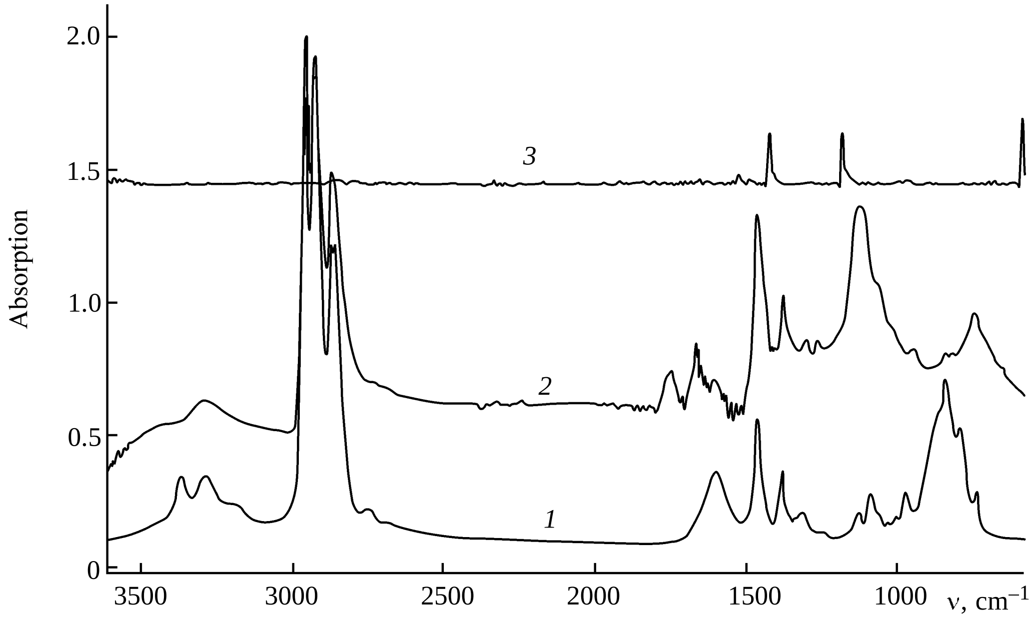


Fig. 2. IR spectrum of (*1*) butylamine, (*2*) A–C_{60} sample, and (*3*) fullerene C_{60}.

constant *K* at the specific concentration of the solution. These data were used for constructing the concentration dependence and extrapolating *K* to the zero concentration. Since for the sample under study the constant *K* was virtually independent of the concentration (Fig. 3b), the experimental *K* parameter for A–C_{60} [$(1.4\pm0.2)\times10^{-10}$ cm^5 g^{-1} (300 V)$^{-2}$] was calculated as an average for the concentrations.

Using the experimentally measured specific increments of the dielectric permittivity [$(\varepsilon - \varepsilon_0)/c = 2.19\pm0.06$] and of the squared refractive index [$(n^2 - n_0^2)/c = 0.323\pm 0.005$], we calculated by relationship (2) the specific dielectric polarization of the sample of A–C_{60} $\mu^2/M = (1.6\pm0.4)\times10^{-38}$ (CGS units).

$$\frac{\mu^2}{M} = \frac{27kT}{4\pi N_A}\frac{1}{(\varepsilon_0^2 + 1)^2}\left[\frac{\varepsilon - \varepsilon_0}{c} - \frac{n^2 - n_0^2}{c}\right]. \qquad (2)$$

Here, μ is the permanent dipole moment; *M*, molecular weight of the object under study; *k*, Boltzmann

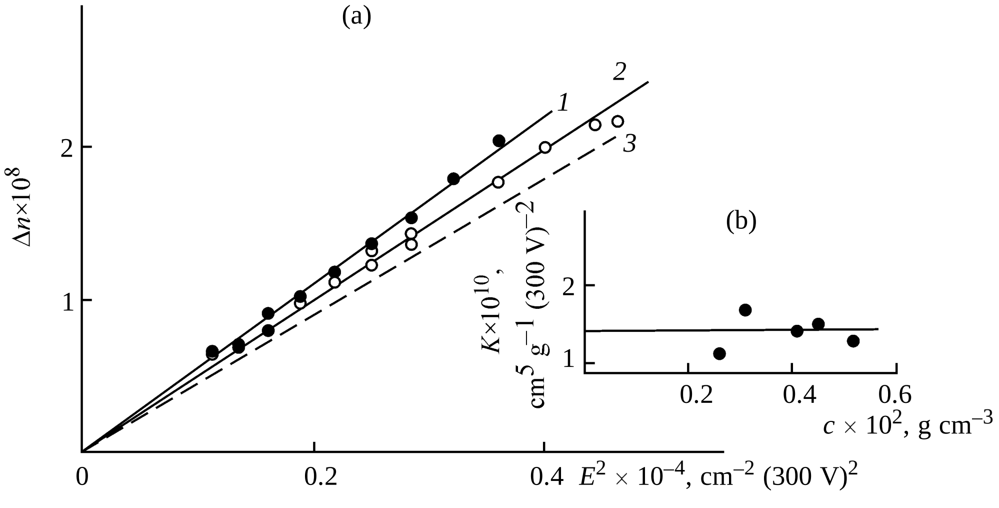
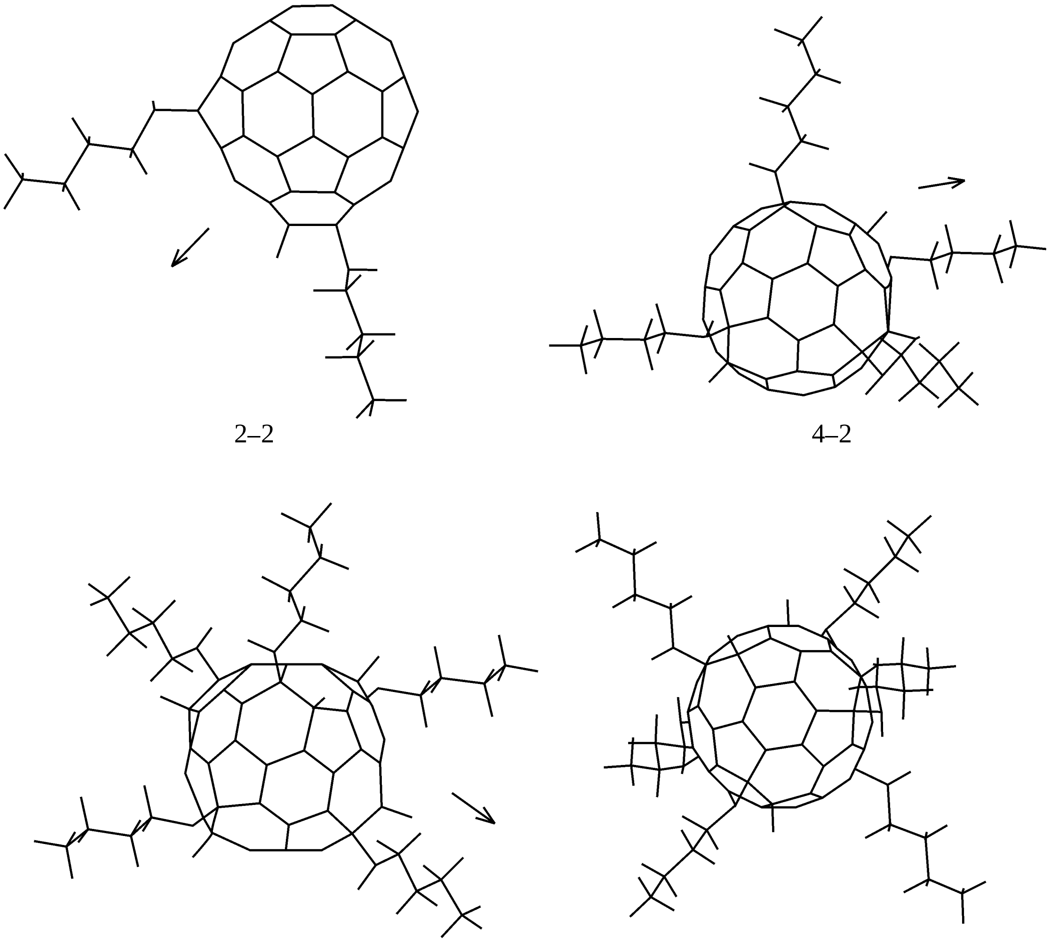


Fig. 3. (a) Variation of Δ*n* with the squared electric field intensity E^2 (*1*, *2*) for A–C_{60} in toluene at the solution concentrations of (*1*) 0.518 and (*2*) 0.311×10^{-2} g cm^{-3} and (*3*) for pure toluene and (b) concentration dependence of *K* for A–C_{60} sample in toluene.


2–2 4–2

5 6

Fig. 4. Structure of the A–C_{60} molecules with the number of amine molecules added $m = 2, 4, 5, 6$ (PM3, MOPAC program; the designations correspond to the numbers of the model A–C_{60} molecules in Table 1; arrows indicate the directions of the permanent dipole moment of the polar structures).

constant; N_A, Avogadro number; T, temperature, K; ε and ε_0, dielectric permittivities of the solution and solvent, respectively; and n and n_0, refractive indices of the solution and solvent, respectively.

The experimental parameters K and μ^2/M of the A–C_{60} sample were compared with the corresponding calculated data, derived from the theoretical molecular parameters of the model molecules of A–C_{60} under assumption that they have 1–6 amine molecules added. Figure 4 presents some of the optimized structures of the A–C_{60} molecules differing in the number of the amine molecules added.

For fully optimized model molecules (with amine molecules added in accordance with the regioselectivity rule for C_{60} [13]) (Fig. 5), we calculated theoretically the eigenvalues of their optical polarizability tensor b_i ($i = 1, 2, 3$) and optical polarizability anisotropy $\Delta b = \{[(b_1 - b_2)^2 + (b_2 - b_3)^2 + (b_3 - b_1)^2]/2\}^{1/2}$, as well as the parameters μ for the varying number m of the arms added to C_{60}. Next, we applied the relationship underlying the Kerr effect theory [formula (3)] for the substances whose molecules can be modeled by rotation ellipsoids with the corresponding symmetry of properties [12, 17] and calculated the molar Kerr constants K_M for these A–C_{60} molecules.

$$K_M = 2\pi N_A(\theta_1 + \theta_2), \tag{3}$$

$$\theta_1 = (45kT)^{-1}[(b_1 - b_2)^2 + (b_2 - b_3)^2 + (b_3 - b_1)^2],$$

$$\theta_2 = (45k^2T^2)^{-1}[(\mu_1^2 - \mu_2^2)(b_1 - b_2) + (\mu_2^2 - \mu_3^2)(b_2 - b_3) + (\mu_3^2 - \mu_1^2)(b_3 - b_1)].$$

Here, θ_1 and θ_2 are contributions from the deformation and orientation components of the Kerr effect, and μ_i, projections of the dipole moment onto the axes of the coordinate system, whose axis 1 corresponds to

Table 1. Parameters *M*, calculated parameters μ and Δ*b* (PM3), and the calculated parameters θ_1 and θ_2 [Eq. (3)], K_M, and μ^2/M for A–C_{60} molecules with different numbers of amine molecules added *m*

m^a	M	μ, D^b	$\Delta b \times 10^{24}$, $cm^{3\,c}$	$\theta_1 \times 10^{34}$	$\theta_2 \times 10^{34}$	$K_M \times 10^{10}$, $cm^5\,(300\ V)^{-2}$	$K_M^{av} \times 10^{10}$, $cm^5\,(300\ V)^{-2\,d}$	$(\mu^2/M) \times 10^{38}$, CGS units
1	793	2.44	10.06	1.108	13.69	55.96	55.96	0.75
2–1	866	0.0008	20.50	4.6	<0.001	17.40	46.67	$\sim 10^{-7}$
2–2		3.37	10.36	1.175	13.01	53.99		1.31
3–1	939	2.32	18.15	3.60	0.67	16.15	20.35	0.57
3–2		4.00	1.63	0.029	7.019	26.66		1.70
4–1	1012	0.001	21.43	5.027	~0.0001	19.01	56.93	$\sim 10^{-7}$
4–2		3.12	10.74	1.26	16.30	66.41		0.96
5	1085	2.12	11.06	1.34	12.44	52.11	52.11	0.39
6	1158	0.003	2.37	0.0615	~0.0001	2.33	2.33	$\sim 10^{-7}$

[a] Designations 1, 2–1, 2–2, 3–1, 3–2, 4–1, 4–2, 5, and 6 correspond to the addition scheme in Fig. 5; [b] $\mu = (\Sigma\mu_i^2)^{1/2}$, $i = 1, 2, 3$. [c] $\Delta b = \{[(b_1 - b_2)^2 + (b_2 - b_3)^2 + (b_3 - b_1)^2]/2\}^{1/2}$. [d] $K_M^{av}(2) = 0.2K_M(2\text{–}1) + 0.8K_M(2\text{–}2)$; $K_M^{av}(3) = 0.6K_M(3\text{–}1) + 0.4K_M(3\text{–}2)$; $K_M^{av}(4) = 0.2K_M(4\text{–}1) + 0.8K_M(4\text{–}2)$.

the largest polarizability of the molecules; other designations are identical to those in Eq. (2).

Tables 1 and 2 present the calculated data and model parameters of the theoretically possible structures of the A–C_{60} molecules at different parameters *m*.

The specific (per unit mass) parameters *K* and K_M are related as (4) [17].

$$K = [(n_0^2 + 2)^2(\varepsilon_0 + 2)^2 K_M]/M \times 6n_0. \qquad (4)$$

Table 1 suggests that the possible, according to the regioselective rule of structures, A–C_{60} adducts with $m = 1$–6 include polar and optically anisotropic (see μ and Δ*b* parameters) nanoparticles whose electrooptical properties will be determined by the contribution from the orientation term θ_2 due to the occurrence of a permanent dipole moment of the particle [see Eq. (3)], since in this case $\theta_2 > \theta_1$, and also virtually nonpolar nanoparticles ($\mu \sim 0$) for which the Kerr effect is due only to anisotropy of their optical polarizability, i.e., to θ_1.

A sharp weakening of the anisotropy of the optical polarizability and dipole moment of A–C_{60} with six arms is due, evidently, to restoration of the symmetry of the molecule, close to that of the initial C_{60}, which though exhibits significant optical polarizability, is nonpolar ($\mu = 0$) and optically isotropic (for eigenvalues of the polarizability tensor of fullerene C_{60} holds $b_1 = b_2 = b_3 = 68.93 \times 10^{-24}$ cm^3, and hence $\Delta b = 0$).

The experimental parameter μ^2/M for the A–C_{60} sample correlates with the calculated data, though does not correspond to any of the theoretically possible structure nos. 1–9, whose characteristics are presented in Table 1. The parameter μ^2/M for the A–C_{60} sample studied is best fit to the most polar of the theoretically calculated adducts of C_{60}. This suggests

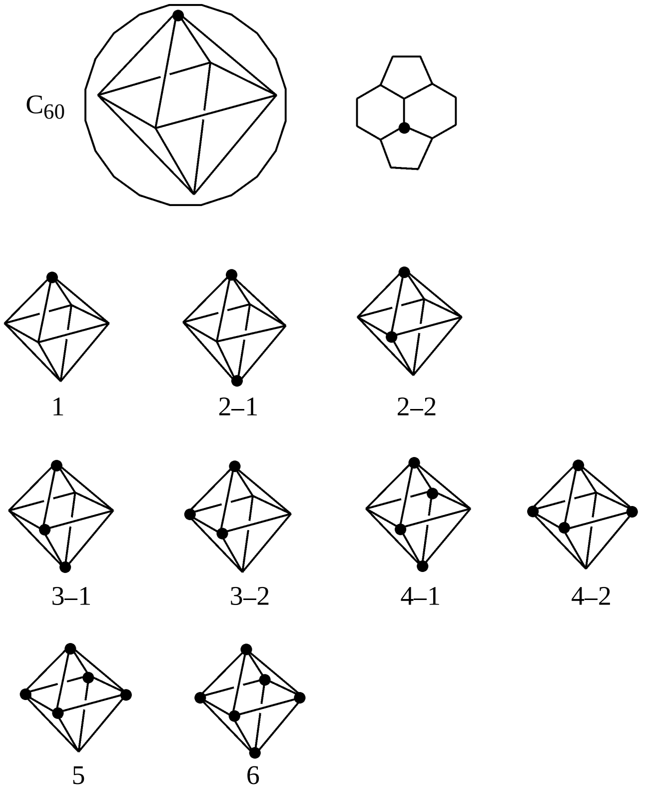


Fig. 5. Regioselective scheme of addition of different numbers of similar groups to fullerene C_{60}, according to [13] (adduct numbers correspond to those of the molecular structures of the A–C_{60} molecules in Table 1).

Table 2. Heats of formation ΔH_f calculated (PM3) for A–C_{60} molecules with different numbers of amine molecules added *m*, heats of formation ΔH_f^{av} averaged for isomeric adducts with identical *m*, and energy gain ΔE from formation of the adducts per A molecule, calculated by formula (5)

m	ΔH_f, kJ mol^{-1}	ΔH_f^{av}, kJ mol^{-1}	ΔE, kJ mol^{-1}
0	3398.4	3398.4	–
1	3197.9	3197.9	–108.9
2	2998.2	2997.2	–108.9
	2996.1		
3	2795.5	2794.3	–109.3
	2793.0		
4	2594.6	2592.9	–109.3
	2591.2		
5	2388.6	2388.6	–110.1
6	2184.7	2184.7	–110.5

unambiguously the presence of polar molecules in the sample. However, the parameter μ^2/M does not exhibit additivity in solutions, and the proportion of polar molecules in A–C_{60} cannot be derived from the experimental μ^2/M parameter. At the same time, the K_M parameter is known [17] to exhibit additivity for inhomogeneous in composition molecular objects in solution, which can be utilized in analysis of the composition of the A–C_{60} sample.

The calculated heats of formation ΔH_f (Table 2) for the structures 2–1 and 2–2, 3–1 and 3–2, 4–1 and 4–2, i.e., for polar and nonpolar isomers with identical numbers of amine molecules added, are very close, which allows formation of polar and nonpolar A–C_{60} adducts to be considered as equally probable events.

The energy gain $\Delta E(m)$ (Table 2) per butylamine molecule, due to formation of adducts of C_{60} with the number of amine molecules added m = 1–6, can be estimated by Eq. (5):

$$\Delta E(m) = \frac{\Delta H_f^{av} - \Delta H_f(0)}{m} - \Delta H_f(A). \qquad (5)$$

Here, $\Delta H_f^{av}(m)$ is the averaged heat of formation $\Delta H_f(m)$ of the isomeric adducts with identical numbers of amine molecules added m; and $\Delta H_f(A)$, heat of formation of butylamine. Calculations show that $\Delta E(m)$ is virtually identical for all the adducts, since the difference in the calculated $\Delta E(m)$ parameters does not exceed the thermal motion energy (2.51 kJ mol^{-1} at room temperature).

The fact that $\Delta E(m)$ is virtually independent of m suggests that the equilibrium constants K_{eq} (6) are identical at m = 0–6.

$$A_m\text{–}C_{60} + A \overset{K_{eq}}{\rightleftarrows} A_{m+1}\text{–}C_{60}. \qquad (6)$$

Then, the numerical fraction $x(m)$ of adducts with m amine molecules added will be described by relationship (7).

$$x(m) = \frac{(K_{eq}[A])^m}{\sum\limits_{m=0}^{m=6}(K_{eq}[A])^m}$$

$$= \begin{cases} 1/7, & (K_{eq}[A] = 1), \\ \dfrac{(K_{eq}[A])^{m+1} - (K_{eq}[A])^m}{(K_{eq}[A])^7 - 1}, & (K_{eq}[A] \neq 1). \end{cases} \qquad (7)$$

The weight fractions of the adducts $w(m)$ were calculated by Eq. (8).

$$w(m) = \frac{x(m)M(m)}{\sum\limits_{m=0}^{m=6} x(m)M(m)}. \qquad (8)$$

Here, $M(m)$ are the molecular weights of the adducts with m amine molecules added (Table 1). The parameter K_M for the sample comprised of adducts with different number of amine molecules added m can be calculated by formula (9).

$$K_m = \sum_{m=0}^{m=6} w(m)K_M^{av}(m). \qquad (9)$$

Formula (9) includes the averaged K_M^{av} parameter (Table 1) for isomeric (polar and nonpolar) adducts with identical m. The reason is equal thermodynamic probability of distribution of the addends A over the fullerene core (the calculated ΔH_f parameters of isomeric adducts are close for identical m, as seen from Table 2). It can be easily demonstrated for such equally probable distribution that, for m = 2, only 3 of 15 possible adducts will have nonpolar structure 2–1 [$K_M^{av}(2) = 0.2K_M(2\text{–}1) + 0.8K_M(2\text{–}2)$]; for m = 3, only 8 of 20 possible adducts will have polar structure 3–2 [$K_M^{av}(3) = 0.6K_M(3\text{–}1) + 0.4K_M(3\text{–}2)$]; and for m = 4, only 3 of 15 possible adducts will have nonpolar structure 4–1 [$K_M^{av}(43) = 0.2K_M(4\text{–}1) + 0.8K_M(4\text{–}2)$].

Calculations by formulas (7–9) using the $K_M^{av}(m)$ parameters from Table 1 show that K_M has a maximum at $K_{eq}[A] \approx 1$, when noticeable contributions come from adducts with both m = 1 and m = 5, having the largest $K_M^{av}(m)$ parameters.

When $K_{eq}[A] = 1$, for all the adducts holds $x(m)$ = 1/7 and $w(0) = 0.11$, $w(1) = 0.12$, $w(2) = 0.13$, $w(3)$ =

0.14, $w(4) = 0.15$, $w(5) = 0.17$, and $w(6) = 0.18$, which yields the calculated K_M parameter of 34×10^{-10} cm^5 (300 V)$^{-2}$.

To estimate K_M from the experimental $K = 1.4 \times 10^{-10}$ cm^5 g^{-1} (300 V)$^{-2}$ for the A–C_{60} sample, we have to set a molecular weight of the sample under study. The number-average and weight-average molecular weights of the adducts at $x(m) = 1/7$ (m = 0–6) were estimated at 939 and 963 g mol^{-1}, respectively. Using Eq. (4), this yields K_M of 38×10^{10} and 37×10^{10} cm^5 (300 V)$^{-2}$, respectively; these values are close to the calculated data.

The equilibrium constant K_{eq} can be estimated from the condition $K_{\text{eq}}[\text{A}] = 1$, taken above. Since fullerene is modified in an over 200-fold molar excess of butylamine (see below), we can take for [A] the concentration of individual butylamine, namely, 10 M (for butylamine $\rho_4^{20} = 0.74$ g cm^{-3}, $M = 73$ g mol^{-1}); then $K_{\text{eq}} \sim 0.1$ l mol^{-1}.

Unfortunately, there are no published data on K_{eq} for reactions of C_{60} with butylamine. However, Ichida *et al.* [18] estimated at 0.02 ± 0.01 l mol^{-1} the equilibrium constant of formation of a charge-transfer complex between C_{60} and aniline. This is by an order of magnitude smaller than $K_{\text{eq}} \sim 0.1$ l mol^{-1}, obtained in this work. Nevertheless, this difference seems reasonable, since butylamine is a much stronger electron donor than such aromatic amine as aniline.

Our results, first, confirm that the K_M parameters can be adequately estimated from the results of quantum chemical calculations of the polarizability tensors and dipole moments of adducts with different numbers of amine molecules added m, and second, suggest a close-to-equilibrium distribution of the adducts over the number of amine molecules added m = 1–6 in the composition of the A–C_{60} sample studied.

Thus, the product of the reaction between fullerene C_{60} and butylamine is a mixture of polar (noncentrosymmetric distribution of the groups added over the fullerene core) and nonpolar (symmetric distribution) of adducts of C_{60} with equally probable number of amine molecules added from 1 to 6. When exposed to electric field in solutions, the polar adducts in the A–C_{60} sample behave as ordinary polar nanoparticles. This suggests that the methods used in this work are suitable for studying the structural features of other amine derivatives of fullerenes, especially for identifuing of their mono, bis, tris, tetrakis, and pentakis adducts.

A practically important outcome of this study is that, in order to shift the equilibrium in the reaction between the primary amine and fullerene toward adducts with larger numbers of the amine molecules added, it is necessary to increase [A]. Since the reaction is run in liquid amine, the concentrations [A] > 10 M can be attained only by changing to amines with a lower molecular weights compared to A. For example, for propylamine ($\rho_4^{20} = 0.719$ g cm^{-3}) [A] is equal to 12.2 M. This allows $K_{\text{eq}}[\text{A}]$ to be increased from 1 (for A) to 1.22 at the same K_{eq} as for A, which yields $x(0) = 0.07$, $x(1) = 0.09$, $x(2) = 0.11$, $x(3) = 0.13$, $x(4) = 0.16$, $x(5) = 0.20$, and $x(6) = 0.24$.

EXPERIMENTAL

The A–C_{60} adducts were synthesized by introducing 0.3 g of C_{60} (99% C_{60}, available from Fullerenovye Tekhnologii, St. Petersburg) into 85 ml of freshly distilled A with stirring of the solution for 48 h at room temperature. Next, A was removed in a vacuum, and the reaction product was vacuum-dried at 50°C to constant weight, whereupon 100 ml of ethanol was added. The resulting solution was filtered, and ethanol was removed in a vacuum. Drying to constant weight yielded 0.3385 g of A–C_{60}.

The ^{13}C NMR spectrum was recorded on a Bruker-DPX (300 MHz) spectrometer in $CDCl_3$. The IR spectra were recorded on a Bruker IFS-88 IR Fourier spectrometer in KBr, and the electronic spectrum, on a Specord M-40 spectrometer in chloroform.

The electrooptical Kerr effect [12], or birefringence, in solutions of A–C_{60} under exposure to external electric field was studied in a rectangular pulse field at the pulse length of 2 ms and voltage supplied to the measurement cell from 0.1 to 1 kV. The measurements were run in a glass cell with parallel plane titanium electrodes 2 cm long, separated by 0.05 cm. The optical birefringence was recorded photoelectrically, using low-frequency modulation of the elliptical light polarization by the compensation procedure [12]. The light source was a He–Ne laser ($\lambda = 6328 \times 10^{-8}$ cm, capacity 1.5 mW); a thin mica plate with the intrinsic phase difference of $0.01 \times 2\pi$ served as compensator. The A–C_{60} solutions were colored, and the measurements were possible only at concentrations under 0.5×10^{-2} g cm^{-3}.

The specific dielectric polarization of the sample μ^2/M was measured in a toluene solution by the Guggenheim–Smith method [11]. The dielectric permittivity of the solutions was measured in an E12-1 device for measuring the capacity by the zero beating method [11]. The measurements were run in a cylindrical titanium capacitor with the intrinsic capacity of 98.6 pF. The refractive indices of the solutions were measured on an IRF-23 refractometer at the wavelength of 5780×10^{-8} cm. For all the parameters of the setup and details of measurement technique, see [19]. The parameter μ^2/M was calculated by formula (2).

The Kerr effect, dielectric permittivity, and refractive indices for A–C_{60} were measured in toluene at 21°C. At this temperature, the solvent had the following characteristics: $\rho_0 = 0.867$ g cm^{-3}, $n_0 = 1.4972$, and $\varepsilon_0 = 2.385$.

Computer simulation of the A–C_{60} molecules with *m* amine molecules added was carried out by PM3 method using the MOPAC routine [14]. For fully optimized structures of the molecules, the optical polarizability tensor and the components of the permanent dipole moment of the molecules were calculated in the coordinate system with the axis corresponding to their largest polarizability.

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