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U.K. Makhmanov^{1,2}, A.X. Shukurov¹, K.N. Musurmonov¹

Optical transition characteristics and aggregation behavior of C₆₀ fullerene in a xylene/ethanol (70:30) Medium

¹*Institute of Ion-Plasma and Laser Technologies, Uzbekistan Academy of Sciences, Tashkent, Uzbekistan, urolmakh@gmail.com;*

²*National University of Uzbekistan named after Mirzo Ulugbek, Tashkent, Uzbekistan*

In this work, the optical transition characteristics, aggregation state, and resulting film morphology of C₆₀ fullerene were investigated in a fixed xylene/ethanol binary medium with a volume ratio of 70:30 at a C₆₀ concentration of 0.1 mg/mL. The system was characterized using UV–Vis absorption spectroscopy, Tauc-type analysis, nanoparticle tracking analysis (NTA), Raman spectroscopy, and atomic force microscopy (AFM). The absorption spectrum shows pronounced ultraviolet and blue-region absorption associated predominantly with electronic transitions of C₆₀. A Tauc-type representation gives characteristic intercept energies near 1.90, 2.13, and 2.88 eV; these values are treated as apparent optical transition energies rather than as independently established band gaps. NTA measurements reveal a broad number-weighted particle-size distribution, with the main particle population located approximately in the 100–200 nm range and an extended low-density tail toward larger sizes. The cumulative size parameters were $D_{10} = 117.8 \pm 15.1$ nm, $D_{50} = 155.2 \pm 9.8$ nm, and $D_{90} = 350.7 \pm 78.9$ nm. Examination of the Raman spectrum identifies characteristic C₆₀ vibrational features while taking into account possible contributions from the xylene/ethanol medium. AFM analysis reveals heterogeneous aggregate-rich film morphology formed after solvent evaporation. The results provide a consistent characterization of C₆₀ under the investigated xylene/ethanol (70:30) condition and establish a basis for further systematic studies of solvent-composition effects.

Keywords: C₆₀ fullerene; xylene/ethanol medium; optical transitions; aggregation; nanoparticle tracking analysis; Raman spectroscopy.

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Introduction

Fullerenes have garnered considerable attention in recent decades due to their outstanding and tunable physical, chemical, and electronic properties [1, 2]. As zero-dimensional (fullerenes) nanostructured carbon allotropes, they possess high symmetry, delocalized π -electron systems, and remarkable stability, making them ideal candidates for a wide range of applications [3-5]. These include the development of advanced materials for optoelectronics, energy conversion, medicine, and nanotechnology. Numerous scientific publications and patented technologies have explored their use in the fabrication of photodetectors, field-effect transistors, supercapacitors, superconductors, drug delivery systems, and nonlinear optical devices [6-8]. Their structural

diversity and electronic tunability open vast possibilities for tailored functional materials.

Among the fullerenes, the C₆₀ molecule stands out due to its high I_h symmetry, well-defined spherical geometry, and unique electronic structure [9]. This molecule consists of 60 carbon atoms arranged in a truncated icosahedron, composed of 12 pentagons and 20 hexagons, resembling a soccer ball. Its π -conjugated surface enables delocalization of electrons, which is key to its chemical reactivity and photo response [10]. C₆₀ displays a range of intriguing physical phenomena, such as photoconductivity, photoinduced electron transfer, and strong light absorption in the ultraviolet-visible region. These features position C₆₀ as a promising material in organic photovoltaic devices, light-harvesting systems, and molecular electronics [11].

A fundamental parameter that governs the optoelectronic behavior of C_{60} is its band gap, i.e., the energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). This band gap plays a decisive role in determining the molecule's optical absorption, electronic conductivity, and chemical activity [12]. In isolated C_{60} molecules, the band gap typically falls in the range of 1.6 to 2.0 eV, which corresponds to absorption in the visible spectral region. This allows fullerene to act as a light-absorbing material in devices requiring semiconducting behavior. The HOMO–LUMO gap also influences electron transport and charge separation in solar energy applications, where C_{60} can act as an efficient electron acceptor [13]. Importantly, the band gap and aggregation behavior of C_{60} are not fixed, but can vary depending on the molecular environment, particularly the solvent system in which the molecule is dispersed [14]. The polarity of the solvent, its dielectric constant, and specific solvation interactions can induce shifts in the HOMO and LUMO energy levels due to electronic stabilization or perturbation effects. Furthermore, C_{60} tends to aggregate in many solvents, especially in those where solubility is low [15]. Aggregation can modify intermolecular electronic interactions and consequently affect the optical absorption profile and apparent transition energies of C_{60} systems [16]. These solvent-induced effects on electronic structure are of practical importance for tailoring fullerene-based systems for specific functions in optoelectronics, sensing, and energy storage.

In this study, we investigate the optical transition characteristics, aggregation state, and resulting film morphology of C_{60} fullerene in a fixed xylene/ethanol binary medium with a volume ratio of 70:30 at a C_{60} concentration of 0.1 mg/mL. The study is intended to establish the optical and colloidal characteristics of C_{60} under this specific mixed-solvent condition rather than to determine a systematic solvent-composition dependence.

I. Experimental

1.1. Used materials.

High-purity crystalline C_{60} fullerene powder ($\geq 99.8\%$) was obtained from Sigma-Aldrich (USA). The solvents used ortho-xylene (C_8H_{10} , referred to as xylene) and ethanol (C_2H_6O) were also of analytical grade and supplied by Sigma-Aldrich. Xylene ($\geq 99.0\%$ purity) and ethanol (96.0% purity) were used without further purification.

1.2. Preparation of fullerene (C_{60}) solutions.

To prepare working solutions of C_{60} fullerene in binary solvents, a molecular solution of C_{60} in xylene was first obtained. Approximately 10 mg of crystalline C_{60} powder was added to 70 mL of xylene and stirred using a programmable magnetic stirrer (MS-11H, WIGO, Poland) at ~ 2.5 Hz for 4 hours in the dark. The resulting solution was then filtered through a $0.22\ \mu\text{m}$ pore-size membrane to remove dust and undissolved particles. Next, 30 mL of ethanol was slowly added to the C_{60} /xylene solution, followed by an additional 1-hour stirring period. This yielded a C_{60} /xylene/ethanol binary solution with a

fullerene concentration of 0.1 mg/mL and a solvent volume ratio of 0.7:0.3 (xylene:ethanol).

1.3. Characterization.

The optical absorption investigations of C_{60} solutions were carried out with a UV–Vis Shimadzu UV-2700 spectrophotometer (Shimadzu, Japan) against a blank solvent. Nanoparticle tracking analysis (NTA) measurements were carried out using a NanoSight LM10 instrument (NanoSight, Amesbury, UK). The system comprised a conventional optical microscope, a Marlin charge-coupled device (CCD) camera, and an LM10 sample chamber equipped with a laser illumination source. NTA was employed to determine the number-weighted particle-size distribution of C_{60} aggregates in the xylene/ethanol (70:30, v/v) medium by tracking the Brownian motion of individual light-scattering particles. The cumulative particle-size parameters D10, D50, and D90 were extracted from the resulting distributions to characterize the size range and polydispersity of the C_{60} aggregates.

The Raman spectra of fullerene solutions were recorded using an InVia Raman spectrometer (Renishaw, UK). A Cobolt CW 532 nm DPSS laser served as the excitation source, operating at a wavelength of 532 nm. In experiments to determine the surface and dimensional characteristics of synthesized nanosized C_{60} aggregates in solutions, a Solver Next atomic force microscope (AFM) with atomic resolution (NT-MDT, Russia) was used.

II. Results and Discussion.

The optical response of C_{60} is sensitive to its molecular environment and aggregation state. In the present study, the absorption, aggregation, and film-forming characteristics of C_{60} are examined specifically in a xylene/ethanol (70:30 v/v) medium. The following discussion therefore focuses on the experimentally observed characteristics of this particular system rather than on a systematic solvent-composition dependence.

Figure 1 presents the absorption spectrum of a C_{60} /xylene/ethanol solution obtained using UV-Vis spectroscopy. The spectrum can be divided into three distinct regions: short-wavelength region (~ 350 – 425 nm), mid-range region (~ 450 – 600 nm), and long-wavelength region (~ 600 – 800 nm).

The absorption is very strong in the short-wavelength region, indicating that the C_{60} /xylene/ethanol solution absorbs ultraviolet and blue light intensely. This strong absorption is likely associated with $\pi \rightarrow \pi^*$ electronic transitions within the fullerene molecules. As the wavelength increases toward the mid-range region (~ 450 – 600 nm), the absorption intensity gradually decreases, suggesting that the solution transmits more visible and near-infrared light. As the wavelength increases into the 450–600 nm region, the absorption intensity decreases and weak spectral features remain. These features may originate from weaker molecular electronic transitions of C_{60} and vibronic contributions, while aggregation-related broadening may also affect the spectral profile. A definitive assignment of individual bands would require complementary spectroscopic or theoretical analysis

(Figure 1).

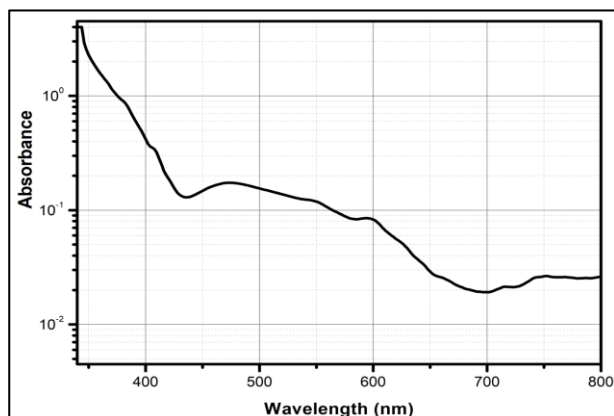


Fig. 1. Absorption spectrum of the C₆₀/xylene/ethanol solution.

Figure 2 demonstrates the optical absorption spectrum of the studied C₆₀/xylene/ethanol solution as a function of photon energy. The vertical axis represents the absorption coefficient, α , expressed in cm⁻¹. The spectrum presents a noticeable increase in absorption with photon energy, indicating electronic transitions characteristic of fullerene molecules. In the lower energy region (approximately 1.5–2.0 eV), absorption remains minimal, suggesting a low density of available electronic states for transition. A gradual increase is observed between 2.0 and 2.8 eV, which can be attributed to $\pi \rightarrow \pi^*$ transitions within the conjugated carbon system of fullerenes. A more pronounced increase in absorption occurs above approximately 3.0 eV, corresponding to higher-energy electronic transitions of C₆₀. A more specific assignment of these transitions would require complementary spectroscopic or theoretical evidence. This behavior is consistent with previously reported optical characteristics of C₆₀ thin films, where absorption increases significantly near the UV region [17]. The spectral profile may additionally be influenced by intermolecular interactions and aggregation of C₆₀ species in the investigated mixed-solvent environment.

A Tauc plot is a graphical method used to estimate the optical band gap of a material from its absorption spectrum, particularly when utilizing UV-Vis or diffuse reflectance spectroscopy [18]. The Tauc relation is expressed as:

$$(\alpha \cdot h \cdot \nu) = A(h \cdot \nu - E_g)^n$$

where A is the absorption constant and $n = 1/2$ for a direct allowed transition. This value of n is appropriate in this case, as the band structure of C₆₀ indicates the presence of a direct electronic transition [19]. For the present analysis, the $(\alpha \cdot h \cdot \nu)^2$ representation was used as a Tauc-type empirical approach corresponding formally to a direct-allowed transition exponent. However, because the investigated system is a molecular/aggregated C₆₀ solution rather than a homogeneous bulk semiconductor, the resulting intercepts are treated only as characteristic optical transition energies.

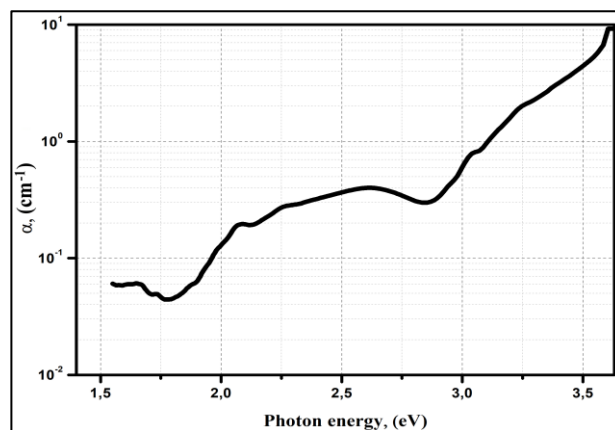


Fig. 2. The absorption coefficient of the C₆₀/xylene/ethanol solution.

The Tauc-type representation shown in Figure 3 contains several approximately linear regions. Linear extrapolation gives characteristic intercept energies near 1.901, 2.130, and 2.880 eV. These values should not be interpreted as three independently established band gaps. Rather, they represent characteristic energies associated with different regions of the optical absorption spectrum and may reflect the contribution of molecular electronic transitions, vibronic structure, and intermolecular interactions within the aggregated C₆₀ system. Because the measurements were performed for a molecular solution at a single solvent composition, assignment of each intercept to a specific electronic mechanism would require additional spectroscopic or theoretical evidence.

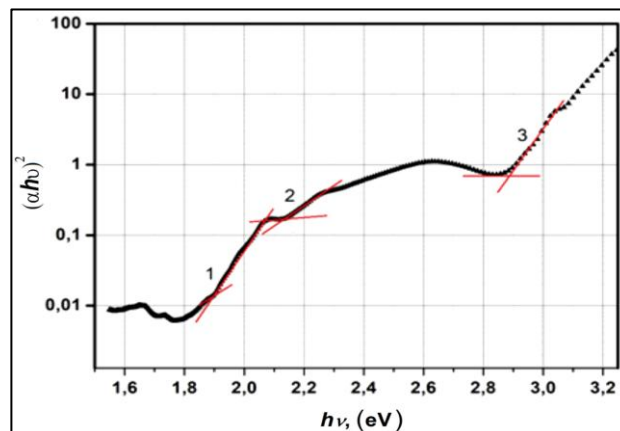


Fig. 3. Tauc-type representation of the optical absorption of C₆₀ in the xylene/ethanol (70:30) medium, showing the selected linear fitting regions. The selected linear fitting regions correspond to characteristic transition energies of 1.901 ± 0.002 , 2.130 ± 0.005 , and 2.880 ± 0.009 eV.

Linear regression was performed for the three approximately linear regions of the Tauc-type representation (Table 1). For Region 1, fitting over 1.9315–2.0130 eV yielded $E_1 = 1.901 \pm 0.0021$ eV with $R^2 = 0.9904$. Region 2, fitted over 2.3308–2.5410 eV, gave $E_2 = 2.130 \pm 0.0046$ eV with $R^2 = 0.9954$. For Region 3, fitting over 2.8704–3.0846 eV resulted in $E_3 = 2.880 \pm 0.0089$ eV with $R^2 = 0.9230$. Thus, the first two regions exhibit very good linearity, whereas the third region shows a noticeably larger deviation from linear

Table 1.

Linear-regression parameters used to determine the characteristic optical transition energies from the Tauc-type representation.

Region	Fitting interval, eV	Slope, m	Intercept, b	E, eV	SE(E), eV	R ²
1	1.9315–2.0130	0.67188	–1.27695	1.901	0.0021	0.9904
2	2.3308–2.5410	2.26200	–4.81778	2.130	0.0046	0.9954
3	2.8704–3.0846	32.6401	–94.0088	2.880	0.0089	0.9230

behavior. Accordingly, the value obtained for Region 3 should be regarded as a less precisely defined characteristic optical transition energy.

Particle-size analysis of C_{60} dispersed in the xylene/ethanol (70:30) medium was performed using nanoparticle tracking analysis (NTA). The resulting size distributions were expressed on a number-weighted basis; therefore, the D_{10} , D_{50} , and D_{90} values represent cumulative particle-size percentiles of the detected particle population rather than intensity-weighted scattering distributions. The corresponding particle-size parameters are summarized in Table 2. All values are reported as mean values with their associated experimental uncertainties, providing a quantitative characterization of the particle-size distribution while accounting for measurement variability. Figure 4 presents the particle number-density distribution, while the cumulative size parameters obtained from repeated measurements are summarized in Table 2.

Table 2.

Cumulative particle-size parameters of the 0.1 mg/mL C_{60} /xylene/ethanol (70:30) solution determined from repeated NTA measurements. Values are presented as mean $\pm$ standard error.

Parameter	Mean $\pm$ standard error, nm
D_{10}	117.8 ± 15.1
D_{50}	155.2 ± 9.8
D_{90}	350.7 ± 78.9

The distribution is relatively broad and asymmetric, with the main particle population concentrated approximately in the 100–200 nm size range. The most pronounced maximum occurs around 150–160 nm, in good agreement with the median particle diameter, $D_{50} = 155.2 \pm 9.8$ nm. A smaller contribution is also visible at sizes close to 100 nm, whereas the distribution gradually decreases toward larger particle sizes and exhibits a low-intensity tail extending to several hundred nanometers. The cumulative NTA parameters provide a quantitative description of this distribution. The D_{10} value of 117.8 ± 15.1 nm indicates that approximately 10% of the detected particles have diameters below this value, whereas $D_{50} = 155.2 \pm 9.8$ nm represents the median particle size. The considerably larger D_{90} value of 350.7 ± 78.9 nm shows that 90% of the detected particles are smaller than approximately 351 nm, while only a relatively small fraction belongs to the larger-size tail. The difference between D_{50} and D_{90} therefore indicates a pronounced broadening of the distribution toward larger hydrodynamic/particle sizes. The substantially larger experimental uncertainty associated with D_{90} also suggests that the upper-size fraction is more variable between repeated measurements than the central part of

the distribution. The NTA results indicate that C_{60} in the xylene/ethanol (70:30) medium exists predominantly as nanoscale aggregates rather than as a monodisperse particle population. The dominant population centered near 150 nm is accompanied by a smaller fraction of larger aggregates, giving rise to the extended distribution tail. Such behavior is consistent with heterogeneous aggregation of C_{60} under the investigated mixed-solvent conditions. However, because only a single solvent composition was examined, the observed size distribution should not be attributed quantitatively to a specific solvent-composition effect without additional comparative measurements.

Figure 5 shows the Raman spectrum recorded for C_{60} in the xylene/ethanol (70:30) medium over the 100–3200 cm^{-1} range. Because the spectrum was measured directly from the solution, it contains contributions from both C_{60} and the solvent components. A band observed near 504.99 cm^{-1} lies close to the well-established $A_g(1)$ radial breathing mode of C_{60} , typically reported near 496 cm^{-1} . The intense band at 1468.53 cm^{-1} agrees well with the characteristic $A_g(2)$ “pentagonal-pinch” mode of C_{60} and provides clear spectroscopic evidence for the presence of intact fullerene molecules. The feature at approximately 733 cm^{-1} is not assigned to the $A_g(1)$ mode; its origin may involve overlapping fullerene and/or solvent contributions and therefore requires cautious interpretation. Similarly, the bands observed in the 2900–3050 cm^{-1} region are predominantly associated with C–H stretching vibrations of the organic solvent components. Consequently, only the reliably assigned fullerene modes are used here for structural interpretation, while the remaining bands are treated as mixed or solvent-related spectral features.

Figure 6 presents 3D and 2D AFM topography images of the dried film prepared from the C_{60} /xylene/ethanol (70:30) solution. The scanned $20 \times 20 \mu\text{m}^2$ area exhibits pronounced surface heterogeneity, including elevated domains, ridge-like features, and isolated aggregates. The maximum vertical height is approximately 1.2 μm . These observations directly demonstrate non-uniform organization of the deposited C_{60} -containing material after solvent evaporation. The observed morphology may be influenced by changes in C_{60} solubility during drying as well as by differences in the physicochemical and evaporation properties of xylene and ethanol. However, because only a single solvent composition was investigated and the evaporation kinetics were not independently measured, the individual contributions of solvent polarity, evaporation rate, and possible phase separation cannot be distinguished from the present AFM data alone.

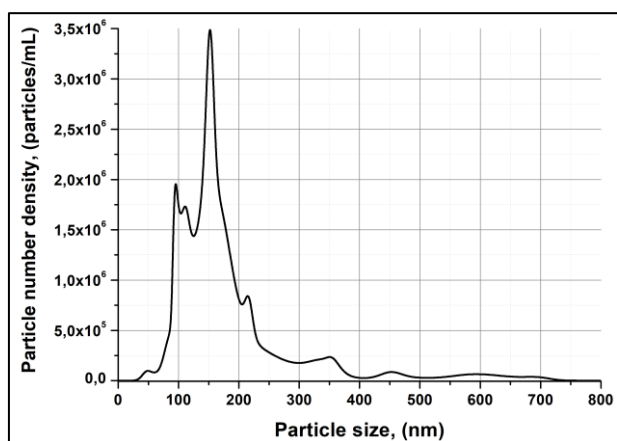


Fig. 4: Number-weighted NTA particle-size distribution of the 0.1 mg/mL C₆₀/xylene/ethanol (70:30) solution.

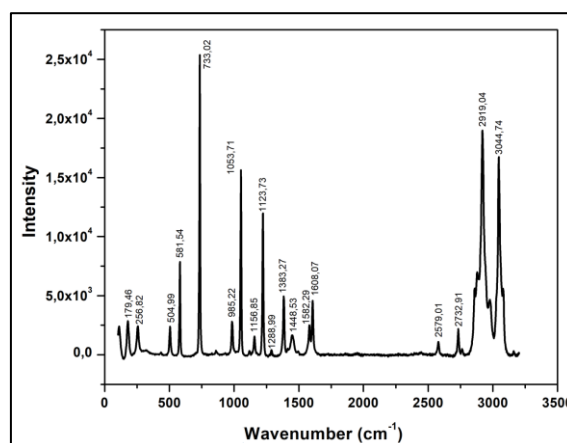


Fig. 5: The Raman spectrum of the C₆₀ fullerene dissolved in a xylene/ethanol (70:30) mixture.

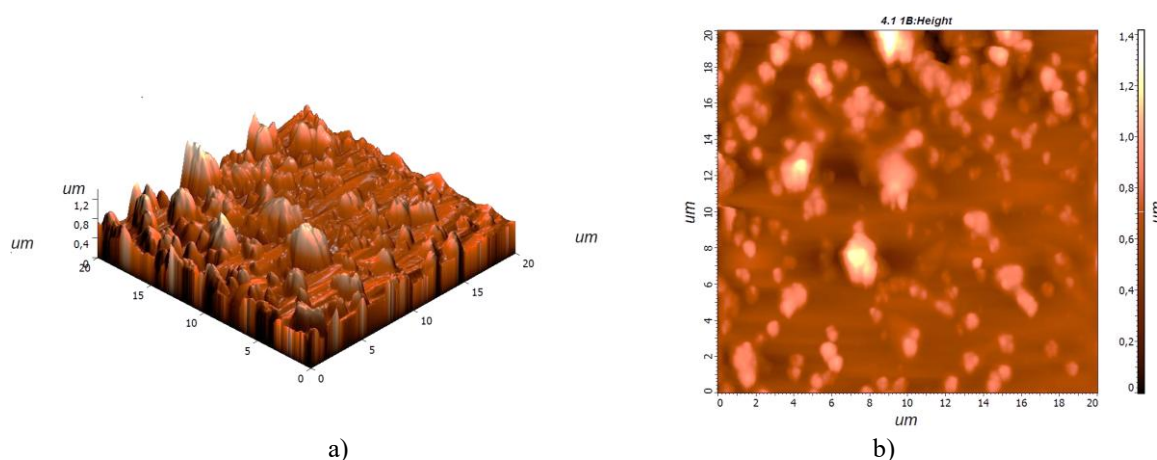


Fig. 6. AFM topography of the dried film prepared from the C₆₀/xylene/ethanol (70:30) solution: (a) 3D and (b) 2D images.

Conclusion

The optical, aggregation, vibrational, and morphological characteristics of C₆₀ fullerene in a fixed xylene/ethanol (70:30 v/v) medium were investigated using UV–Vis spectroscopy, Tauc-type analysis, nanoparticle tracking analysis (NTA), Raman spectroscopy, and AFM. The UV–Vis spectrum shows pronounced absorption in the ultraviolet and blue spectral regions. A Tauc-type representation yields characteristic intercept energies near 1.90, 2.13, and 2.88 eV; these values are interpreted as apparent optical transition energies rather than as three independently established optical band gaps.

NTA measurements revealed a broad number-weighted particle-size distribution dominated by nanoscale aggregates in the approximately 100–200 nm range. The cumulative particle-size parameters D₁₀, D₅₀, and D₉₀ were 117.8 ± 15.1 , 155.2 ± 9.8 , and 350.7 ± 78.9 nm, respectively. The substantially larger D₉₀ value reflects an asymmetric distribution with a relatively small fraction of larger aggregates extending toward several hundred nanometers.

Examination of the Raman spectrum confirms that the band near 1469 cm⁻¹ corresponds to the characteristic

A_g(2) pentagonal-pinch mode of C₆₀, whereas the lower-frequency A_g(1) breathing mode occurs near the 496–505 cm⁻¹ region. Solvent-related contributions are considered explicitly in the interpretation of the remaining bands.

AFM imaging reveals a heterogeneous film surface containing aggregated C₆₀ domains formed after solvent evaporation. Variations in solubility and solvent-evaporation behavior may contribute to the observed morphology, although the present measurements do not allow a systematic solvent-composition effect to be established. Overall, the study provides an experimental characterization of the optical and aggregation behavior of C₆₀ under the specific 70:30 xylene/ethanol condition.

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Makhmanov U.K. – Doctor of Physical and Mathematical Sciences, Professor, Head of the Laboratory;
Shukurov A.X. – PhD in Physics and Mathematics, Senior researcher;
Musurmonov K.N. – Junior researcher.

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У.Дж. Махманов^{1,2}, А.Х. Шукуров¹, К.Н. Мусурмонов¹

Характеристики оптичних переходів та особливості агрегації фулерену C₆₀ у середовищі ксилол/етанол (70:30)

¹ Інститут іонно-плазмових і лазерних технологій Академії наук Узбекистану, Ташкент, Узбекистан, urolmakh@gmail.com;

² Національний університет Узбекистану імені Мірзо Улугбека, Ташкент, Узбекистан

У роботі досліджено характеристики оптичних переходів, стан агрегації та морфологію утворених плівок фулерену C₆₀ у бінарному середовищі ксилол/етанол із фіксованим об'ємним співвідношенням 70:30 за концентрації C₆₀ 0,1 мг/мл. Для характеристики системи використано спектроскопію поглинання в УФ–видимій області (UV–Vis), аналіз за методом Тауца, аналіз траєкторій наночастинок (NTA), раманівську спектроскопію та атомно-силову мікроскопію (АСМ). Спектр поглинання демонструє виражене поглинання в ультрафіолетовій та синій областях спектра, пов'язане переважно з електронними переходами у C₆₀. Представлення даних у координатах Тауца дає характерні енергії перетину поблизу 1,90, 2,13 та 2,88 еВ; ці значення розглядаються як ефективні енергії оптичних переходів, а не як незалежно встановлені значення ширини забороненої зони. Вимірювання методом NTA виявили широкий розподіл частинок за розмірами, зважений за їх кількість, причому основна популяція частинок перебуває приблизно в діапазоні 100–200 нм, а розподіл характеризується протяжним низькоінтенсивним «хвостом» у напрямку більших розмірів. Кумулятивні параметри розподілу за розмірами становили: D10 = 117,8 ± 15,1 нм, D50 = 155,2 ± 9,8 нм та D90 = 350,7 ± 78,9 нм. Аналіз раманівського спектра дозволив ідентифікувати характерні коливальні моди C₆₀ з урахуванням можливого внеску середовища ксилол/етанол. За результатами АСМ-аналізу встановлено неоднорідну морфологію плівки зі значною кількістю агрегатів, що формується після випаровування розчинника. Отримані результати забезпечують комплексну характеристику C₆₀ у досліджуваному середовищі ксилол/етанол (70:30) та створюють основу для подальших систематичних досліджень впливу складу розчинника.

Ключові слова: фулерен C₆₀; середовище ксилол/етанол; оптичні переходи; агрегація; аналіз траєкторій наночастинок; раманівська спектроскопія.