ОПТИКА И ЛАЗЕРНАЯ ФИЗИКА

TIME EVOLUTION OF THE OPTICAL AND STRUCTURAL PROPERTIES OF C_{70} FULLERENE IN BENZENE–CYCLOHEXANE SOLVENTS

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In this study, we comprehensively investigated the aggregation processes of fullerene C_{70} in a benzene/cyclohexane binary solution, taking into account the effects of concentration and time. The optical properties of the samples were analyzed using UV-visible and Raman spectroscopy, as well as refractometry (n and BRIX parameters). The preservation of the positions of specific maxima of C_{70} unchanged in the UV-visible spectra indicates that the aggregation process does not disturb the fundamental electronic structure of the molecule. Raman analysis showed that the increase in the intensity of some vibrational modes and a decrease in the number of peaks over time are associated with physical clustering processes. Refractometric results showed that the refractive index increases with increasing C_{70} concentration. Although the UV–Vis absorption intensity continues to increase up to the 20th day, the refractive index and BRIX values exhibit only minor variations in the 15–20 day interval, indicating that the system approaches a dynamic optical equilibrium in terms of refractometric response. It was noted that aggregation occurs faster in the sample with a higher concentration.

Keywords: C_{70} fullerene, benzene–cyclohexane solutions, UV–Vis spectroscopy, Raman spectroscopy, aggregation, refractive index.

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Introduction. At present, carbon-based nanostructures, including fullerenes, carbon nanotubes, graphene, and other carbon allotropes, are considered among the most promising materials in modern materials science, nanophotonics, quantum optics, biomedicine, and sensor technologies [1]. The unique properties of this class of materials are directly related to their spatial geometry, highly delocalized π-electron system, degree of symmetry, and intermolecular interactions [2]. In particular, fullerenes are distinguished by their ability to effectively modulate optical, electronic, and vibrational processes due to their specific geometry, multielectron resonance system, and characteristic electron–phonon coupling mechanisms [3].

Among the fullerene family, the C_{70} molecule has an ellipsoidal shape, which leads to additional splitting of electronic energy levels, increased orbital degeneracy lifting, and, as a result, richer optical and Raman spectra [4]. The relatively lower symmetry of C_{70} causes an expansion of the range of electronic transitions, less sharply defined energy level separations, and increased sensitivity to the surrounding environment. Therefore, C_{70}-based systems serve as a convenient model for studying light absorption, luminescence, photocurrent processes, and electronic relaxation mechanisms in dispersed media.

The physical behavior of C_{70} molecules in solution is a multifactorial process that strongly depends on solvent polarity, aromatic or inert character, concentration, aggregation kinetics, time, and the strength of dispersive intermolecular interactions [5–7]. π–π interactions, van der Waals forces, dispersive interactions, and slow intermolecular dynamic fluctuations in the solvent environment lead to redistribution of the electronic density of C_{70} molecules. These effects manifest in noticeable spectral changes, such as red or blue shifts of absorption maxima in UV–Vis spectra, narrowing or broadening of Raman bands, and variations in their intensities [8].

Nonpolar organic solvents such as benzene and cyclohexane are considered suitable media for the stable dispersion of C_{70} in liquid systems. The aromatic ring of benzene forms resonant π–π interactions with the π-electron cloud of C_{70}, activating the electronic environment in solution and increasing the probability of certain electronic transitions [9]. Cyclohexane, in contrast, is relatively inert, providing structural stability in solution and acting as a passive medium during aggregation processes [10]...

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