Self-assembly of tartrazine molecules in water-dimethylsulphoxide solution

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Abstract. Spectroscopic and theoretical calculations have shown that the self-aggregation of tartrazine molecules occurs in an aqueous and water-dimethylsulphoxide solution with a hypochromic effect in their electronic spectra. The deformation of the absorption spectra is accompanied by long-wave broadening. The absorption band of the dye E102 self-aggregates corresponds to the maxima \( \lambda_{\text{max}} = 463 \text{nm} \) and \( \lambda_{\text{max}} = 483 \text{nm} \). Studies of the linear dichroism spectra have established that tartrazine self-aggregates, which have a needle-like structure, have optical activity. These data are the passport characteristics of self-assembled tartrazine molecules and they can be used to determine the nativity of dye self-aggregates. It is established that by selecting the concentration and ratios of binary solvent mixtures, it is possible to regulate the number of molecules in the self-aggregated dye molecules. The integration of tartrazine molecules into self-aggregates occurs by Van der Waals forces.

1. Introduction
In food and pharmaceutical practice, both natural and synthetic dyes are widely used [1]. Synthetic dyes have some advantages over natural dyes. Because they give bright, easily reproducible colors that are resistant to light, temperature, oxidants, reducing agents, PH changes and are less sensitive to various types of influences that the material is exposed to in the technological process. The yellow dye tartrazine (E102) is one of the synthetic, water-soluble dyes [2]. A number of authors have experimentally and clinically shown that tartrazine can induce hypersensitivity of the body, which is regarded as side effects when staining drugs or vitamins [3-5]. Despite the fact that some authorities have long banned the use of tartrazine as a dye for coloring medicines and food products (Order of the Minister of the Ministry of Health of the Russian Federation No. 8 of 19.03.1998), there are still reports in scientific publications about the detection of traces of this dye in the bodies of children and adult patients [5-7]. Taking into account the toxicity of the dye, in clinical studies, a number of authors were able to develop methods for removing or reducing the amount of tartrazine in the patient's body[8-12]. When developing a method for reducing the amount of tartrazine in the body, they were based on the study of electronic bands, IR spectra and the results of microscopic studies of the affected part of the body. However, the authors of these studies did not take into account the possibility of self-aggregation or complex formation of tartrazine molecules in the form of their nanoparticles [16]. In these cases, the detection and removal of dye molecules from the body is relevant. These studies allow us to find out not only the nature of the electronic transition as a result of self-aggregation of molecules, but also determine the nature of the interaction force in the formation of their nanoparticles.
By definition, self-assembly is a process in which only the components of the final structure participate. Combinations of molecules in solutions can be carried out under the influence of various intermolecular interactions (MMV). The appearance of MMV contributes to the self-assembly of solute molecules. This process is accompanied by a significant deformation of the spectral-optical characteristics of the compound under study \[17,18\]. Elucidating the nature of the forces that cause the self-assembly of molecules is one of the most pressing problems in the physics of the modern condensed state.

The purpose of this study was to identify the conditions for self-aggregation of dye E102 using solvents approved by the Ministry of Health (water and dimethylsulfoxide) for their use in medical practice. Determine the position of the electronic absorption bands of dimers and complex aggregates. These bands can serve as passport characteristics of dimeric and complex self-aggregates of dye molecules. Based on these bands, clinical researchers can evaluate the nativity of self-aggregated molecules.

2. Experimental method

In the work, the powder of the food dye tartrazine (E-102) was used. The electronic absorption spectra were measured using a Specord 50 SA spectrophotometer (Analytikjena, Germany), which allows optical density measurements in the range of 190-1100nm. The optical rotation dispersion and linear dichroism spectra were recorded on a Jasko-20 dichrograph with an optical attachment of a double Fresnel parallelepiped used in the visible and UV parts of the spectral region.

The solvent used was bidistilled water, dimethylsulfoxide (DMSO) purified according to known methods \[19\]. Microscopic studies were carried out on a biological microscope KSO 5001-1 “Anjeon presicion optics Co, Hd” (South Korea) and on an electron microscope (SEM) TESCAN Mira3 (Russia).

The quantum-chemical calculation of the electronic structure and charge distribution on the atoms of tartrazine molecules was carried out using the MOPAC 2009 software package using the semi-empirical AM1 method with a standard set of parameters \[20, 21\].

Binary solvent mixtures were prepared in such a way that the concentration of the compound under study remained constant, and the ratio of the binary solvent mixture changed. In the second case, the composition of the binary solvent mixture remained constant, and the dye concentration changed.

The frequency of the pure electronic transition (v00) was determined using the rule of mirror symmetry of the absorption spectra, the rule of V. L. Levshin \[22\]. Another method of determination (v00) is based on the universal ratio of B. I. Stepanov between the absorption and luminescence spectra.

\[
\frac{I_\nu}{\nu^2 \epsilon_\nu} = C \frac{h(v_{00}-\nu)}{kT}
\]

where \(I_\nu, \epsilon_\nu\) are the emission power in relative units and the extinction coefficient, respectively, at the selected temperature. \(h, K\) are the Planck and Boltzmann constants, respectively.

3. Results and discussion

3.1. Spectroscopic studies of self-aggregation of tartrazine molecules

The self-assembly of tartrazine was studied in water and water-dimethylsulfoxide solutions. The choice of solvent was due to the fact that water and dimethylsulfoxide are used in medical practice as a cryoprotector and it is added to the cell environment to prevent cell damage from freezing. 10% DMSO solutions can also be used to safely cool the cell, and it is used dimethylsulfoxide is used as an anti-inflammatory and analgesic agent \[23\].

First of all, we studied the absorption spectrum of tartrazine in water. At the same time, it was found that in the spectrum of the long-wave absorption band, a maximum with \(\lambda_{\text{max}}=426\text{nm}\) is observed. Moreover, the shape and intensity of the dye spectrum in a wide concentration range of \(5 \cdot 10^{6} \div 10^{4}\)M
practically remain unchanged, and they relate to the absorption capacity of monomeric tartrazine molecules (figure 1 and cur.11 figure 1a) of the test compound. To simplify the discussion of the results obtained, the absorption spectra were normalized to one. As can be seen from figure 1a, as the concentration of the aqueous solution increases, there is a drop in the absorption capacity (hypochromic effect) with a broadening of the absorption spectrum with respect to the bands of monomers of tartrazine molecules (Curves 2-5 of figure 1a).

For a detailed study of the self-assembly of tartrazine molecules, we conducted experiments in binary mixtures of water-dimethylsulphoxide (water-DMSO) solution. Figure 1b shows the absorption spectra of tartrazine at a constant concentration (C=5·10⁻⁶ M) with a change in the proportion of water in the water-dimethylsulphoxide solution. It was experimentally established that the absorption spectrum in 100% water coincides with the band of a low-concentrated aqueous solution that belongs to monomeric dye molecules. As the water fraction decreases and the volume of DMSO increases at a constant concentration, the absorption capacity of the solution with the hypochromic effect decreases (figure 1b Curve 2-3). In this case, the absorption bands in the long-wavelength part of the spectrum of monomers of tartrazine molecules are widened. The deformation of the spectra is accompanied by the formation of an isobestic point (λ₁=463nm). Such a change in the absorption spectra is associated with the formation of tartrazine self-aggregates in the form of dimers. In this case, both monomeric and dimeric tartrazine molecules will be in the solutions. A further increase in the proportion of DMSO in binary solutions leads to an increased drop in the absorption capacity with the appearance of a second isobestic point (λ₂=513nm) (figure 1b curve 4-8).

A further increase in the dye concentration leads to the formation of opalescence of the solution, and it becomes cloudy, colloidal.

An increase in the temperature of the water+DMSO solution leads to the restoration of the electron bands characteristic of monomeric tartrazine molecules. An increase in the temperature of the solution to 80-85°C leads to a complete restoration of the absorption bands of monomeric tartrazine molecules. The binding energies of self-assembled dye molecules in binary solvent mixtures were determined from temperature experiments based on the method [24]. The value of these energies was 22-24 kJ/mol, which corresponds to the energy of the hydrogen bond.

![Figure 1](image_url)

**Figure 1.** Concentration dependence of the absorption spectra of tartrazine in water. (a) - C=5·10⁻⁶ (1), 10⁻⁵(2), 5·10⁻⁵(3), 10⁻⁴(4), 5·10⁻⁴(5) M (1-5); and a binary mixture of water-DMSO concentration C=5·10⁻⁶ M of the water content (b) - 100%(1), 80%(2), 60%(3) 40%(4), 30%(5), 20%(6), 10% (7), 5%(8).
Aggregation in the water+DMSO binary mixture for tartrazine molecules can be explained as follows. When tartrazine is dissolved in water, each molecule will be surrounded by solvate shells of the solvent. In this case, the intermolecular interaction (MMV) directly between the molecules of the dissolved compound is excluded and they are in the monomeric state. The addition of the second component (DMSO) in which tartrazine is not soluble may lead to the fact that these components are combined with each other according to the scheme: R1O...HR2, where R1 and R2 are the lagging part of the water and dimethylsulfoxide molecules, respectively. As a result of these MMV, the solvate envelope around the solute weakens.

In this case, the molecules of the compound under study leave the solvate shell, as a result of which there is a possibility of interaction between the molecules of the dissolved compounds. These processes lead to the formation of a local volume with a high concentration of the compound under study, as a result of which the molecules are combined in the form of an aggregate. At the first stage of self-aggregation, dimers with absorption bands are formed, which form an isobestic point with $\lambda=463$ nm (figure 1b). As the proportion of dimethylsulfoxide increases, the process of aggregation of tartrazine molecules increases and more complex aggregates are formed with an isobestic point $\lambda=513$ nm (figure 1b). The formation of self-aggregates is confirmed by temperature studies. When the solution temperature reaches a value of 75-85°C, the spectrum of monomeric dye molecules is restored. The binding energy of 22-24 kJ / mol refers to the hydrogen bond energy between the components of a binary solvent mixture (water-DMSO). The combination of tartrazine molecules is carried out by Van der Waals forces, which is confirmed by the theoretical calculations.

3.2. Results and discussions of theoretical calculations

Figure 2a shows the charge distribution, as well as the bond length between dimethylsulfoxide atoms. From figure 2a it follows that the oxygen O1 in dimethylsulfoxide with the H6 and H10 hydrogens have the same bond length $l=1.114$ Å (dotted line) (figure 2a). Also, the same bond lengths are with oxygen O1 with hydrogen H7 and H9 with a bond length $l=1.112$ Å which are equivalent. We assume that intramolecular hydrogen bonds with H6 and H10 and H7 and H9 hydrogens may be formed between the oxygen O1 DMSO. In these cases, the probability of intramolecular hydrogen bonding is realized with the O1 hydrogens H6 and H10. That is, equivalent hydrogen bonds are interactions with H7 and H9 hydrogens. Along with intramolecular hydrogen bonds, the oxygen DMSO O1 is also bound to the hydrogen H2 and H3 of water molecules. These connections are equivalent. Moreover, the bond of oxygen O1 with water hydrogens is equivalent and the structure of aggregates between these molecules is shown in figure 2b. The theoretical values of the binding energy (water-DMSO) $E=5.32$ kCal/mol, which corresponds to 22.34 kJ/mol.

![Figure 2](image.png)

**Figure 2.** Structures of the monomeric form of DMSO (a) and self-aggregates of dimethylsulfoxide with water (b).
As a result of theoretical calculations, it shows that the self-assembly of tartrazine molecules is carried out in concentrated aqueous and binary solvents water+DMSO. In this case, the binding energy with values of 22-24 kJ/mol refers to binary mixtures of water+dimethylsulfaxide solvents. At the same time, the tartrazine molecules are combined by Van der Waals forces.

3.3. Absorption bands of tartrazine self-aggregates

From the above experimental results, it follows that in aqueous and aqueous dimethylsulfaxide solutions, the apparent absorption band of self-assembled tartrazine molecules is practically not manifested (figure 1b). However, a long-wave broadening of the spectrum of monomeric tartrazine molecules is observed. In order to identify the absorption bands of dimers of tartrazine molecules, we normalized (figure 1 with a curve.3 figure 1b) refers to the monomers and dimeric dye molecules, respectively, where the process of dimerization of tartrazine molecules occurs with an isobestic point of wavelength $\lambda=485\text{nm}$. From the algebraic sums according to the method [25], the Lorentz sums were distinguished in the form of curves 9-10 in figure 3a. In this case, curve 9 was assigned to the absorption band of dimeric dye molecules, which corresponds to a maximum wavelength of $\lambda=485\text{nm}$, and curve 10 was assigned to the absorption band of dimethylsulfaxide with a maximum wavelength of $\lambda=276\text{nm}$ [26]. Similarly, the absorption bands of complex aggregates of tartrazine molecules were determined. In these cases, the bands were compared (curve1 c 8 figure 1b) with an isobestic point $\lambda=513\text{nm}$. Also, according to the Lorentz components, the bands were allocated (curves 11-12 of figure 3b). Curve 11 was assigned to the band of complex aggregates of tartrazine and curve 12 was assigned to the absorption band of dimethylsulfaxide with a wavelength of $\lambda=276\text{nm}$. The hypochromic effect of self-aggregates of tartrazine molecules is apparently due to the fact that, the intensity of the absorption capacity of dimers and complex self-aggregates. Approximately an order of magnitude less in relation to the intensity of the absorption capacity of monomeric molecules of tartrazine. The shape and maximum of the absorption rods of dimers and complex self-aggregates of tartrazine molecules are confirmed by the images of the linear dichroism spectra, where the formation of tartrazine self-aggregates can also occur.

Figure. 3. The absorption spectrum of monomers (1) and dimer (3) (figure 1b) and their algebraic sum 9-10 (a); and (1) and (8) (figure 1b) and their algebraic sum 11-12(b) of tartrazine molecules.
From the analysis of the literature data, it follows that linear dichroism spectroscopy turned out to be a very informative and accurate method for controlling the degree of self-assembled molecules in the medium. To obtain sufficient information, the authors measured the spectra of self-assembled aggregated molecules from the spectra of linear dichroism along the non-chiratron rotation of the polarization plane.

We found that in the case when self-assembled tartrazine molecules of the compound under study are formed in the solution and pumping such a solution through a flow cell leads to the appearance of linear dichroism. In this case, the orientation of the self-assembled aggregated molecules is carried out by pumping the corresponding solution through a millimeter cuvette at a speed of 2 mm/s. The experimental pumping speed of the solution was chosen in such a way as to provide a laminar hydrodynamic flow and it was oriented at an angle of 45° to the polarization of the linear polarized light incident on the cuvette. It is also experimentally established that only when self-assembly of aggregated molecules is formed or a colloidal solution occurs under the conditions of flow of these solutions through a flow cell, they become optical anisotropic. Apparently, only when the combined dye molecules are partially oriented in the hydrodynamic laminar molasses, they will turn out to be anisotropic and the linear dichroism of the solution is manifested. Only in this case, the dichrograph registers the curve of the linear dichroism spectrum from the zero line [27].

We have studied solutions of self-assembled tartrazine molecules obtained under laminar hydrodynamic flow conditions. At the same time, it was found that they exhibit a significant linear dichroism, its value in the maximum of the absorption band at $\nu=23500 \text{ cm}^{-1}$ is $\Delta D_{\parallel,\perp}=10^{-2}$ units.

![Figure 4](image)

**Figure 4.** Linear dichroism spectra of self-assembled tartrazine molecules under hydrodynamic flow of its aqueous solution at the angle between the flow velocity vector and the polarization vector of the transmitted light $+45^0$ (1) and $-45^0$ (2). The self-assembled dye bands (3) and its Lorentz components (4,5) $C = 5 \times 10^{-5}$M, $l = 0.1$ cm.

The algebraic sum of the spectral curves 1 and 2 gives a curve 3 of which, by applying the Lorentzian contour decomposition. Using the method [28], two different amplitude bands of linear dichroism were identified, the position of the maxima $\lambda_{1}=463\text{nm}$ and $\lambda_{2}=485\text{nm}$, which coincides with the bands of aggregates obtained from the absorption spectra (figure 9, figure 3a) and (curve.11 figure 3b). The fact that the tartrazine associates exhibit linear dichroism, easily navigating in the laminar hydrodynamic flow, indicates a strong anisotropy of the dye microcrystals, which have a needle-like (rod-shaped) shape. Thus, the absorption of self-aggregates of tartrazine molecules is determined by two methods (the absorption spectra and the linear dichroism spectra coincide with each other).
3.4. Energy of electronic transitions of monomers and self-aggregates of tartrazine molecules

The energy parameters of the electronic transition in monomers and self-aggregates are determined from the electronic absorption and linear dichroism spectra. For the monomeric form of tartrazine molecules, the most likely frequency transitions in the absorption ($\nu_p$) are: $\nu_m = 23700$ cm$^{-1}$, in the dimer $\nu_d = 21600$ cm$^{-1}$, complex aggregates $\nu_c = 20600$ sm$^{-1}$. The frequency of the pure electronic transition is determined by two methods [28]. Results the frequency of the purely electronic transition $\nu_0$ for the monomer molecules tartrazine $\nu_m = 23700$ cm$^{-1}$, dimer $\nu_d = 21600$ sm$^{-1}$ for complex units $\nu_c = 19800$ sm$^{-1}$.

Based on the values of the maxima of the absorption bands and linear dichroism, schemes of electronic transitions between the ground and excited states of tartrazine in the monomeric and aggregated states were constructed (figure 5).

![Figure 5. Scheme of electronic transition frequencies of monomers (a), dimers (b) and complex self-aggregates (v) of tartrazine molecules.](image)

It follows from figure 5 that the frequencies of the purely electronic transition for dimers with respect to monomeric molecules decrease by 2·1000 cm$^{-1}$. For complex self-aggregates, this value is 3·1000 cm$^{-1}$.

Comparison of the process of self-aggregates of tartrazine obtained in aqueous and water-dimethylsulphoxide solutions shows that, regardless of the orientation of monomeric molecules, self-aggregation of tartrazine molecules occurs. In these cases, in the electronic levels of monomeric molecules in the excited state, the resonant splitting of the excited electronic levels occurs.

For a dimeric unit cell in a molecular crystal, the following relation is satisfied in the dipole-dipole interaction between monomer molecules:

$$\Delta E_D = \Delta E_M + \Delta D + V_{12}$$

where $\Delta E_D$ and $\Delta E_M$ are the electron transition energies in the dimer and monomer, respectively; $\Delta D$ - the difference in the interaction energy of the excited and normal monomer molecules with another monomer molecule in the dimer unit cell of the dye aggregate.
The energy of the exciton interaction between monomer molecules in the dimeric unit cell of the tartrazine aggregate $V_{12} = 3000 \text{ cm}^{-1}$, which is characteristic of the strong dipole-dipole bonds between molecules observed in crystals of molecular nature. The resonant exciton lifetime in such a molecular crystal was determined from the ratio $t = h/2V_{12}$. For a dimeric unit cell of a vitamin preparation, it is of the order of $3 \times 10^{-16} \text{ s}$. This is typical for a free exciton whose resonant lifetime is shorter than the relaxation time of the lattice of a molecular crystal. The rate of excitation transfer between molecules in a dimeric unit cell (the resonance rate) is $n = 1/t = 3 \times 10^{15} \text{ s}^{-1}$. It also follows from figure 5 that the difference in the energy of interaction between the excited and normal molecules in the dimeric unit cell of the tartrazine aggregate $\Delta D = +2000 \text{ cm}^{-1}$. The shift of the center of the exciton absorption band of the aggregate in relation to the absorption band of the monomeric form of tartrazine in the red region of the spectrum is due to the fact that the interaction energy between the molecules in the dimeric unit cell in the ground state is greater than in the excited state.

4. Conclusions
It was found that tartrazine molecules in concentrated aqueous solutions and in an aqueous-dimethylsulfoxide solution form aggregates with a hypochromic effect and optical activity. The hypochromic effect of the absorption spectrum is due to the fact that the intensity of the absorption capacity of self-aggregates is an order of magnitude less than the intensity of monomeric tartrazine molecules, which are also taken into account in clinical studies. It is shown that the tartrazine molecules combine as a result of a strong dipole-dipole interaction. As a result, there is a resonant splitting of the excited levels of the electronic state of dimeric and complex self-aggregates of tartrazine molecules.

According to the linear dichroism spectra, it was determined that tartrazine self-aggregates have a needle-like structure. By selecting the concentration and composition of binary solvent mixtures, the number of molecules in the dye E102 self-aggregates can be adjusted.

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