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STATISTICAL CALCULATION OF THE VISCOSITY COEFFICIENTS OF THE ORDERED PHASES OF DNA MOLECULES

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Statistical calculation of the viscosity coefficients of the ordered phases of DNA molecules is performed. As a starting point of calculation, an expression which describes the tensor of viscous stresses is used, whereas calculations of time correlation functions that determine kinetic coefficients are performed with the aid of a relaxation equation which characterizes the evolution of the tensor order parameter.

Physically, the ordered phases revealed experimentally in the DNA molecule are interesting biological objects [1]. They represent concentrated solutions of the fragments of DNA molecules with the length close to their persistent length in ionic media formed by aqueous salt solutions. The latter possess a liquid-crystalline orientational order responsible for their anisotropy.

Orientational Order and Its Kinetics for the Ordered DNA Molecules. Since condensed states of the ensembles of DNA molecules have a liquid-crystalline orientational order, its description in both nematic and cholesteric liquid crystals should be made using an average value of the dynamic density of the tensor order parameter in the form of a spurless second-order tensor (see. e.g., [2]):

$$D_{ij}(\mathbf{x}) = \frac{1}{2} \sum_{v=1}^N (3c_i^v c_j^v - \delta_{ij}) \delta(\mathbf{x} - \mathbf{x}^v). \tag{1}$$

The dynamic parameter of the density of the tensor order parameter is a nonconserved quantity, and therefore its evolution obeys the relaxation equation [2]:

$$\frac{d\hat{\delta}D_{ij}}{dt} = - \sum_{\alpha=1}^3 \tau_{\alpha}^{-1} B_{ijkl}^{\alpha} \hat{\delta}D_{kl}, \tag{2}$$

with $\hat{\delta}D_{ij} = \hat{D}_{ij} - D_{ij}^0$ representing the deviation of the tensor parameter from its equilibrium value D_{ij}^0 .

The time correlation function of the tensor order parameter is determined in the form of integrals over the volume of the system with the aid of the relation

$$g_{ijkl}(t) = \frac{1}{V} \iint \langle \hat{\delta}D_{ij}(\mathbf{x}, t) \hat{\delta}D_{kl}(\mathbf{x}', 0) \rangle d\mathbf{x}d\mathbf{x}', \tag{3}$$

in which the angular brackets denote equilibrium averaging. Since the equation of motion for the time correlation function $g_{ijkl}(t)$ coincides with the equation of the temporal evolution of the dynamic quantity $\hat{\delta}D_{ij}(t)$, an equation for $g_{ijkl}(t)$ can be written in the form

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$$\frac{d}{dt} g_{ijkl}(t) = - \sum_{\alpha=1}^3 \tau_{\alpha}^{-1} B_{ijmn}^{\alpha} g_{mnkl}(t). \quad (4)$$

The structure of the tensor $g_{ijkl}(t)$, because of the uniaxial symmetry of the medium and the fact that $D_{ii} = 0$, is determined by the expression

$$g_{ijkl}(t) = \sum_{\alpha=1}^3 g_{\alpha}(t) B_{ijkl}^{\alpha}. \quad (5)$$

The coefficients $g_{\alpha}(t)$ obey three independent equations. The unknown correlation function has the form

$$g_{ijkl}(t) = \sum_{\alpha=1}^3 g_{\alpha}(0) \exp\left(-\frac{t}{\tau_{\alpha}}\right) B_{ijkl}^{\alpha}. \quad (6)$$

The independent coefficients $g_{\alpha}(0)$ define the static correlation function

$$g_{ijkl}(0) = \frac{1}{V} \iint \langle \hat{D}_{ij}(\mathbf{x}, 0) \hat{D}_{kl}(\mathbf{x}', 0) \rangle d\mathbf{x} d\mathbf{x}', \quad (7)$$

represented by the expression

$$g_{ijkl}(0) = \sum_{\alpha=1}^3 g_{\alpha}(0) B_{ijkl}^{\alpha}. \quad (8)$$

For the coefficients $g_{\alpha}(t)$ in [2], formulas in the form of average values of the cosines and sines of the angle θ between the axis of a fragment of a DNA molecule and director are derived.

The times of relaxation of the orientational order τ_{α} are determined with the aid of the formulas

$$\tau_{\alpha} = \frac{g_{\alpha}(0)}{F_{\alpha}}, \quad (9)$$

where F_{α} are the independent coefficients of the tensor

$$F_{ijkl} = \sum_{\alpha=1}^3 F_{\alpha} B_{ijkl}^{\alpha}. \quad (10)$$

The tensor considered can be represented in terms of integrals of the following form:

$$F_{ijkl} = \frac{1}{V} \int d\mathbf{x} \int d\mathbf{x}' \int_0^t dt \exp(-\varepsilon t) \langle \hat{I}_{ij}^D(\mathbf{x}, t) \hat{I}_{kl}^D(\mathbf{x}', 0) \rangle,$$

with $\hat{I}_{ij}^D(\mathbf{x}, t)$ being a source in the equation of motion for microscopic tensor order parameters $\hat{D}_{ij}(\mathbf{x}, t)$ [2].

Calculation of the tensor of the kinetic coefficients F_{ijkl} is performed approximately with the aid of the Fokker-Planck equation for a single-particle function of the distribution of orientational variables [2]. The result of calculation can be presented in the form

$$F_1 = \frac{9nkT}{4\xi} \left(1 - \overline{\cos^4 \theta}\right), \quad F_2 = \frac{27nkT}{2\xi} \left(\overline{\cos^2 \theta} - \overline{\cos^4 \theta}\right), \quad F_3 = \frac{9nkT}{2\xi} \left(1 - 3\overline{\cos^2 \theta} + 4\overline{\cos^4 \theta}\right). \quad (11)$$

According to the Einstein formula, the coefficient of rotational friction ξ is expressed in terms of the coefficient of rotational diffusion:

$$D = \frac{kT}{\xi}. \quad (12)$$

On the other hand, the coefficient D can be calculated from the hydrodynamic formula [3]

$$D = \frac{kT}{6\eta\Omega\delta}. \quad (13)$$

If the ratio of the length of the molecule to its diameter $L_p/d = 100$, then $\delta = 721$ [3], whereas at $L_p/d = 25$, $\delta = 62.8$. For the DNA molecule, it is characteristic that $L_p/d = 25$, which corresponds to $L_p = 500$ Å (persistent length) and diameter $d = 20$ Å. We note that "hydrodynamic" formula (13) corresponds to the results of the statistical model [4]. Thus, the times of relaxation τ_α have been determined on the basis of the statistical theory.

We recall [2] that τ_1 is the time of relaxation of biaxial fluctuations, τ_2 is the time of relaxation of longitudinal fluctuations of ordering, and τ_3 is the time of relaxation of transverse uniaxial fluctuations. It is of importance that in transition to the homogeneous state (degenerate as concerns the orientation of the director) of a nematic liquid crystal the quantity τ_3 goes to infinity, and then the components of the ordering parameter D_{23} and D_{13} describe the so-called Goldstone hydrodynamic modes. If the degeneracy considered is removed by external fields or by the action of boundary conditions that create orientating forces, then τ_3 is finite.

The formulas for τ_α can be presented in the form [2]

$$\tau_1 = \tau \frac{7 - 10\bar{P}_2 + 3\bar{P}_4}{7 - 5\bar{P}_2 - 2\bar{P}_4}, \quad \tau_2 = \tau \frac{7 + 10\bar{P}_2 + 18\bar{P}_4 - 35\bar{P}_2}{7 + 5\bar{P}_2 - 12\bar{P}_4}, \quad \tau_3 = \tau \frac{7 + 5\bar{P}_2 - 12\bar{P}_4}{14 + 5\bar{P}_2 + 16\bar{P}_4}. \quad (14)$$

Here $\tau = (6D)^{-1}$, whereas \bar{P}_2 and \bar{P}_4 are average values of the Legendre polynomials expressed in terms of $\cos \theta$:

$$\overline{\cos^2 \theta} = \frac{1}{3}(1 + 2\bar{P}_2), \quad \overline{\cos^4 \theta} = \frac{1}{35}(7 + 20\bar{P}_2 + 8\bar{P}_4). \quad (15)$$

For subsequent calculations, the average values of $\overline{\cos^2 \theta}$ and $\overline{\cos^4 \theta}$ will be determined in the approximation of the molecular field from the formulas

$$\overline{\cos^2 \theta} = \frac{1}{3}(2s + 1), \quad \overline{\cos^4 \theta} = \frac{1}{3}(2s + 1) - \frac{2}{3b}. \quad (16)$$

Determination of the Viscosity Coefficients for the Ordered Phases of DNA Molecules. For statistical-mechanical description of the viscous properties of condensed systems in terms of the contemporary statistical nonequilibrium theory [5] it is necessary to use an equation for the microscopic tensor of stresses $\hat{\tau}_{ij}(\mathbf{x})$. An expression for this tensor was established earlier [1, 6] and it has the form

$$\hat{\tau}_{ij}(\mathbf{x}) = - \sum_{\nu=1}^N \left(\frac{1}{m} p_i^\nu p_j^\nu + \frac{1}{2} \sum_{\mu \neq \nu}^N F_i^{\nu\mu} X_j^{\nu\mu} \right) \delta(\mathbf{x} - \mathbf{x}^\nu). \quad (17)$$

The specificity of concentrated solutions containing rod-like macromolecules leads to the necessity of introducing a simplified relation for the microscopic tensor of stresses. Such equations that take into account the orientational degrees of freedom were suggested in [6–8]. In what follows, we will use the following expression:

$$\hat{\tau}_{ij} = 3kT \frac{p^2 - 1}{p^2 + 1} \left(c_i c_j - \frac{1}{3} \delta_{ij} \right) + \left(\frac{p^2}{p^2 + 1} c_i \frac{\partial U}{\partial c_j} - \frac{1}{p^2 + 1} c_j \frac{\partial U}{\partial c_i} \right). \quad (18)$$

The single-particle microscopic tensor of stresses $\hat{\tau}_{ij}(\mathbf{x})$ will be represented as a sum of symmetrical and antisymmetrical parts:

$$\hat{\tau}_{ij}(\mathbf{x}) = \hat{\tau}_{ij}^s(\mathbf{x}) + \hat{\tau}_{ij}^a(\mathbf{x}), \quad (19)$$

with

$$\hat{\tau}_{ij}^s = 3kT\chi \left(c_i c_j - \frac{1}{3} \delta_{ij} \right) + \frac{1}{2} \chi \left(c_i \frac{\partial U}{\partial c_j} + c_j \frac{\partial U}{\partial c_i} \right), \quad (20)$$

$$\hat{\tau}_{ij}^a = \frac{1}{2} \left(c_i \frac{\partial U}{\partial c_j} - c_j \frac{\partial U}{\partial c_i} \right), \quad (21)$$

where $\chi = (p^2 - 1)/(p^2 + 1)$ is the quantity characterizing the degree of elongation of a molecule (of a fragment of a DNA molecule). As the potential U we will use its expression in the approximation of the molecular field:

$$U = -\frac{3}{2} kTbs \cos^2 \theta. \quad (22)$$

Having calculated the derivatives of potential (22), we will write down the relationship

$$c_i \frac{\partial U}{\partial c_j} + c_j \frac{\partial U}{\partial c_i} = -3kTbs (c_i c_j n_i n_j + c_j c_i n_i n_j). \quad (23)$$

Resorting to the formula below for the single-particle tensor order parameter:

$$\hat{d}_{ij} = \frac{1}{2} (3c_i c_j - \delta_{ij}), \quad (24)$$

we will represent (23) in the form

$$c_i \frac{\partial U}{\partial c_j} + c_j \frac{\partial U}{\partial c_i} = -2kTbs (\hat{d}_{ij} n_i n_j + \hat{d}_{ji} n_i n_j + n_i n_j). \quad (25)$$

The derivatives that determine the antisymmetric part of the tensor of stresses (21) are calculated in a similar way. As a result, we obtain the relationship

$$c_i \frac{\partial U}{\partial c_j} - c_j \frac{\partial U}{\partial c_i} = -2kTbs (\hat{d}_{ij} n_i n_j - \hat{d}_{ji} n_i n_j). \quad (26)$$

Based on Eqs. (25) and (26), we determine the dynamic value of the total tensor of stresses as the sum of its symmetrical and antisymmetrical parts:

$$\begin{aligned} \hat{\tau}_{ij} = & 2kT\chi \sum_{v=1}^N \hat{d}_{ij}^v \delta(\mathbf{x} - \mathbf{x}^v) + kTbs\chi \left[\sum_{v=1}^N \hat{d}_{ij}^v \delta(\mathbf{x} - \mathbf{x}^v) n_i n_j + \sum_{v=1}^N \hat{d}_{ji}^v \delta(\mathbf{x} - \mathbf{x}^v) n_i n_j \right] + \\ & + kTbs \left[\sum_{v=1}^N \hat{d}_{ij}^v \delta(\mathbf{x} - \mathbf{x}^v) n_j n_i - \sum_{v=1}^N \hat{d}_{ji}^v \delta(\mathbf{x} - \mathbf{x}^v) n_i n_j \right]. \end{aligned} \quad (27)$$

In deriving Eq. (27), summation was made over the number of particles, with each term being multiplied by $\delta(\mathbf{x} - \mathbf{x}^v)$.

Using the expression for the density of the dynamic value of the tensor order parameter:

$$\hat{D}_{ij}(\mathbf{x}) = \sum_{v=1}^N d_{ij}^v \delta(\mathbf{x} - \mathbf{x}^v) = \sum_{v=1}^N \frac{1}{2} (3c_i^v c_j^v - \delta_{ij}) \delta(\mathbf{x} - \mathbf{x}^v), \quad (28)$$

we write down the density of the dynamic value of the microscopic tensor of stresses in the form

$$\hat{\tau}_{ij}(\mathbf{x}) = 2kT\chi\hat{D}_{ij}(\mathbf{x}) - kT\chi bs (\hat{D}_{il}n_l n_j + \hat{D}_{jl}n_l n_i) - kTbs (\hat{D}_{il}n_l n_j - \hat{D}_{jl}n_l n_i) \quad (29)$$

or

$$\hat{\tau}_{ij}(\mathbf{x}) = 2kT\chi\hat{D}_{ij} - kTbs (\chi + 1) n_j n_l \hat{D}_{li} - kTbs (\chi - 1) n_l n_i \hat{D}_{lj}. \quad (30)$$

As a result of nonequilibrium averaging (30), the value of the tensor of stresses is determined in terms of the density of the tensor order parameters:

$$\tau_{ij} = 2kTD_{ij} - kTbs (\chi + 1) n_j n_l D_{li} - kTbs (\chi - 1) n_l n_i D_{lj}. \quad (31)$$

However, the nonequilibrium average value of D_{ij} consists of the sum of the equilibrium value D_{ij}^0 and nonequilibrium addition:

$$D_{ij} = D_{ij}^0 + K_{ijkl} \beta \dot{\epsilon}_{kl}, \quad (32)$$

where

$$\dot{\epsilon}_{kl} = \frac{\partial v_k}{\partial x_l} - e_{mlk} \omega_m. \quad (33)$$

The equilibrium value of the tensor order parameter

$$D_{ij}^0 = \frac{1}{2} sn (3n_i n_j - \delta_{ij}) \quad (34)$$

determines the equilibrium portion of the tensor of stresses τ_{ij}^0 . At the same time, the nonequilibrium addition $K_{ijkl} \beta \dot{\epsilon}_{kl}$ in the quantity D_{ij} is proportional to the deformation-rate tensor. On substitution of this addition into expression (31), we establish a linear relationship between the nonlinear tensor of stresses and the tensor of deformation rates. The proportionality factors in the relation indicated form a tensor of the viscosity coefficients of the media studied.

The constitutive equation for the tensor of viscous stresses is written in the form

$$\tau_{ij} - \tau_{ij}^0 = [(\chi\delta_{ij} - bs (\chi + 1) n_j n_l) K_{limn} + (\chi\delta_{ij} - bs (\chi - 1) n_l n_i) K_{ljmn}] \dot{\epsilon}_{mn}. \quad (35)$$

We will denote the tensor of the viscosity coefficients by a_{ijkl} ; then

$$a_{ijkl} = 2\chi K_{ijkl} - bs (\chi + 1) n_j n_m K_{mikl} - bs (\chi - 1) n_l n_m K_{mjkl}. \quad (36)$$

In this approach, computation of the viscosity coefficients is reduced to calculation of the tensor K_{ijkl} which, according to (32), determines the nonequilibrium contribution to the tensor order parameter. Relation (32) results from averaging of the tensor parameter with the aid of the nonequilibrium distribution function [2, 5]:

$$f = f_0 + \sum \int_{-\infty}^0 dx' \int dt' \exp [(\epsilon + (1 - P_M) iL) t'] f_0^m(\mathbf{x}') X_m(\mathbf{x}', t + t'). \quad (37)$$

Among the dynamic values of irreversible flows \hat{j}^m there is a microscopic tensor of stresses, i.e.,

$$\hat{j}^m = (1 - P_M) \hat{\tau}_{ij}. \quad (38)$$

In (37), the conjugated thermodynamic force X_m is equal to $\beta \hat{\epsilon}_{ik}$. We note that f_0 is the equilibrium function of distribution and P_M is the Mori projection operator. In what follows, for the homogeneous case considered, the Liouville operator $(1 - P_M)L$ is reduced to a conventional operator L , with the parameter $\epsilon \rightarrow 0$ after the thermodynamic limiting transition.

An expression for the tensor K_{ijkl} is derived by performing the above-mentioned nonequilibrium averaging \hat{D}_{ij} with the aid of the distribution function (37):

$$K_{ijkl} = \int d\mathbf{x}' \int_0^\infty \exp(\epsilon\tau) \langle \hat{D}_{ij}(\mathbf{x}', \tau) \hat{\tau}_{kl}(0) \rangle d\tau. \quad (39)$$

However, according to (30), the microscopic tensor of stresses is expressed in terms of the dynamic value of the tensor order parameter. Ultimately, computation of the tensor K_{ijkl} is reduced to calculation of integrals of the time correlation function of the tensor order parameter:

$$\begin{aligned} K_{ijkl} = & \left[\int d\mathbf{x}' \int_0^\infty \exp(\epsilon\tau) \langle \hat{D}_{ij}(\tau) \hat{D}_{mk} \rangle d\tau \right] kT (\chi \delta_{lm} - bs (\chi + 1) n_l n_m) + \\ & + \left[\int d\mathbf{x}' \int_0^\infty \exp(\epsilon\tau) \langle \hat{D}_{ij}(\tau) \hat{D}_{ml} \rangle d\tau \right] kT (\chi \delta_{km} - bs (\chi - 1) n_k n_m). \end{aligned} \quad (40)$$

Calculation of the integrals considered is made on the basis of the explicit relation for the above-established time correlation function:

$$g_{ijkl}(t) = \sum_{\alpha=1}^3 g_\alpha(t) B_{ijkl}^\alpha, \quad g_\alpha(t) = g_\alpha(0) \exp\left(-\frac{t}{\tau_\alpha}\right) \quad (41)$$

As a result, the tensor K_{ijkl} can be represented in the form

$$K_{ijkl} = kT (\chi \delta_{lm} - bs (\chi + 1) n_l n_m) \sum g_\alpha(0) \tau_\alpha B_{ijmk}^\alpha + kT (\chi \delta_{km} - bs (\chi - 1) n_k n_m) \sum g_\alpha(0) \tau_\alpha B_{ijml}^\alpha. \quad (42)$$

To simplify the representation, in what follows we introduce the notation

$$b_\alpha = g_\alpha(0) \tau_\alpha. \quad (43)$$

Substituting the tensor K_{ijkl} (42) into the expression for the viscosity coefficients (36), we obtain the following formula:

$$\begin{aligned} \frac{a_{ijkl}}{kT} = & 4\chi^2 \sum b_\alpha B_{ijkl}^\alpha - 2bs\chi (\chi + 1) (n_l n_m \sum b_\alpha B_{ijkl}^\alpha + n_n n_j \sum b_\alpha B_{ijjk}^\alpha) - 2bs\chi (\chi - 1) \times \\ & \times (n_k n_m \sum b_\alpha B_{ijml}^\alpha + n_l n_n \sum b_\alpha B_{njkl}^\alpha) + bs^2 (\chi^2 - 1) (n_j n_m n_n n_k \sum b_\alpha B_{imml}^\alpha + n_l n_n n_l n_m \sum b_\alpha B_{njmk}^\alpha) + \\ & + bs^2 (\chi + 1)^2 n_j n_l n_m n_n \sum b_\alpha B_{imkn}^\alpha + bs^2 (\chi - 1)^2 n_l n_n n_l n_m \sum b_\alpha B_{njml}^\alpha. \end{aligned} \quad (44)$$

Using the explicit form of the Stratanovich matrices, we can represent the tensor $\sum b_\alpha \beta_{ijkl}^\alpha$ in (44) in the form

$$\begin{aligned} \Sigma b_\alpha B_{ijkl}^\alpha &= b_1 B_{ijkl}^{(1)} + b_2 B_{ijkl}^{(2)} + b_3 B_{ijkl}^{(3)} = \left(\frac{b_2}{6} - \frac{b_1}{2}\right) \delta_{ij} \delta_{kl} + \frac{b_1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \\ &+ \left(\frac{b_1}{2} - \frac{b_2}{2}\right) (\delta_{ij} n_k n_l + \delta_{kl} n_i n_j) + \left(\frac{b_3}{2} - \frac{b_1}{2}\right) (\delta_{il} n_j n_k + \delta_{ik} n_j n_l + \delta_{jl} n_i n_k + \delta_{jk} n_i n_l) + \left(\frac{b_1}{2} + \frac{3b_2}{2} - 2b_3\right) n_i n_j n_k n_l. \end{aligned}$$

Then the explicit expression for the tensor of the viscosity coefficients can be written as

$$\begin{aligned} \frac{a_{ijkl}}{kT} &= 2\chi^2 \left(\frac{b_2}{3} - b_1\right) \delta_{ij} \delta_{kl} + 2\chi^2 b_1 \delta_{ik} \delta_{jl} + 2\chi^2 b_1 \delta_{il} \delta_{jk} + 2\chi^2 \left(b_1 - b_2 \left(1 - \frac{2bs}{3}\right)\right) (\delta_{ij} n_k n_l + \delta_{kl} n_i n_j) + \\ &+ 2 \left(\chi^2 (b_3 - b_1) + \left(\frac{bs^2}{4} (\chi + 1)^2 - bs\chi (\chi + 1)\right) b_3\right) \delta_{ik} n_j n_l + 2 \left(\chi^2 (b_3 - b_1) + (bs^2 (\chi^2 - 1) - bs\chi^2) b_3\right) \times \\ &\times (\delta_{il} n_j n_k + \delta_{jk} n_i n_l) + 2 \left(\chi^2 (b_3 - b_1) + \left(\frac{bs^2}{4} (\chi - 1)^2 - bs\chi (\chi - 1)\right) b_3\right) \times \\ &\times \delta_{jl} n_i n_k + 2\chi^2 \left((b_1 + 3b_2 - 4b_3) + bs^2 \left(\frac{4b_2}{3} - b_3\right) - 4bs (b_2 - b_3)\right) n_i n_j n_k n_l. \end{aligned} \quad (45)$$

We will take into consideration that for a uniaxial centrosymmetrical medium the tensor a_{ijkl} has the following structure [2]:

$$\begin{aligned} a_{ijkl} &= a_1 \delta_{ij} \delta_{kl} + a_2 \delta_{ik} \delta_{jl} + a_3 \delta_{il} \delta_{jk} + a_4 (\delta_{ij} n_k n_l + \delta_{kl} n_i n_j) + \\ &+ a_5 \delta_{ik} n_j n_l + a_6 (\delta_{il} n_j n_k + \delta_{jk} n_i n_l) + a_7 \delta_{jl} n_i n_k + a_8 n_i n_j n_k n_l. \end{aligned} \quad (46)$$

On the basis of relation (45) we derive formulas for the viscosity coefficients:

$$\begin{aligned} a_1 &= 2kT\chi^2 \left(\frac{b_2}{3} - b_1\right), \quad a_2 = a_3 = 2kT\chi^2 b_1, \quad a_4 = 2kT\chi^2 \left(b_1 - b_2 \left(1 - \frac{2bs}{3}\right)\right), \\ a_5 &= 2kT \left(\chi^2 (b_3 - b_1) + \left(\frac{bs^2}{4} (\chi + 1)^2 - bs\chi (\chi + 1)\right) b_3\right), \quad a_6 = 2kT \left(\chi^2 (b_3 - b_1) + (bs^2 (\chi^2 - 1) - bs\chi^2) b_3\right), \\ a_7 &= 2kT \left(\chi^2 (b_3 - b_1) + \left(\frac{bs^2}{4} (\chi - 1)^2 - bs\chi (\chi - 1)\right) b_3\right), \\ a_8 &= 2\chi^2 \left((b_1 + 3b_2 - 4b_3) + bs^2 \left(\frac{4b_2}{3} - b_3\right) - 4bs (b_2 - b_3)\right). \end{aligned} \quad (47)$$

In view of the lack of any data on the viscosity and kinetic parameters of the systems investigated, there is a pressing need to determine the indicated quantities on the basis of the theory developed.

To estimate the coefficients of rotational diffusion, we will use hydrodynamic formula (13). The volume of a fragment of the molecule $\Omega = \pi r^2 L_p$ is calculated from the persistent length and $L_p = 500 \text{ \AA}$ and the cross-section radius $r = 10 \text{ \AA}$. As a result, we obtain $\Omega = 1.571 \cdot 10^{-25} \text{ m}^3$. Since the form-factor is equal to 62.8 and water viscosity is $\eta = 10^{-3} \text{ Pa}\cdot\text{sec}$, then at $T = 300 \text{ K}$ and $D = 1.099 \cdot 10^5 \text{ sec}^{-1}$. The relaxation times are calculated from formulas (14), where the average values of the Legendre polynomials are determined with the aid of formulas (15) and (16). Then

$$\tau_1 = \frac{1 - s - \frac{1}{b}}{4D \left(1 - s + \frac{1}{b}\right)}, \quad \tau_2 = \frac{\left(1 + s - 2s^2 - \frac{3}{b}\right)b}{12D}, \quad \tau_3 = \frac{1}{2bD \left(2 + s - \frac{4}{b}\right)}.$$

At $s = 0.5$, we obtain that $\tau_1 = 0.865 \cdot 10^{-6}$ sec, $\tau_2 = 1.169 \cdot 10^{-6}$ sec, and $\tau_3 = 0.619 \cdot 10^{-6}$ sec. Single-particle expressions for g_α are written on the basis of [2] in the form

$$g_1 = \frac{9}{16} n \sin^4 \theta, \quad g_2 = \frac{27}{8} n \left(\overline{\cos^4 \theta} - \overline{\cos^2 \theta}\right), \quad g_3 = \frac{9}{4} n \left(\overline{\cos^2 \theta} - \overline{\cos^4 \theta}\right)$$

or subject to (16) for $\overline{\cos^2 \theta}$ and $\overline{\cos^4 \theta}$ in the form

$$g_1 = \frac{3n}{8} \left(1 - s - \frac{1}{b}\right), \quad g_2 = \frac{3n}{4} \left(1 + s - 2s^2 - \frac{3}{b}\right), \quad g_3 = \frac{3n}{2b}.$$

For numerical estimations we assume that $b = 4.5415$ and $s = 0.5$. The density of the number of DNA molecule fragments will be calculated from the formula $n = \rho/m$. Here m is the mass of a fragment of the molecule and $\rho = (10\text{--}300) \text{ kg/m}^3$ is its mass density. At the same time, the mass of the molecule fragment, the length of which is equal to the persistent one, is determined as $m = 147m_b$, where m_b is the mass of a pair of nitrogen bases, and 147 is their number layed out on the persistent length. Since $m_b = (615 \cdot 10^{-3})/(6.02 \cdot 10^{23}) = 1.02 \cdot 10^{-24} \text{ kg}$ (615 g is the molecular mass, $6.02 \cdot 10^{23}$ is the Avogadro number), as a result $m = 1.5 \cdot 10^{-22} \text{ kg}$.

In what follows, the estimation will be made at $n = 150/(1.5 \cdot 10^{-22}) = 10^{24} \text{ m}^{-3}$ assuming that $\rho = 150 \text{ kg/m}^3$. As a result, we obtain that $g_1 = 0.1033 \cdot 10^{24} \text{ m}^{-3}$, $g_2 = 0.2546 \cdot 10^{24} \text{ m}^{-3}$, and $g_3 = 0.3303 \cdot 10^{24} \text{ m}^{-3}$ and the parameters b_α from (43) are equal to $b_1 = 0.8936 \cdot 10^{17}$, $b_2 = 0.3479 \cdot 10^{18}$, and $b_3 = 0.2044 \cdot 10^{18}$. For the ordered phase of DNA molecules, fragments of length of the order of the persistent one $L_p \approx 500 \text{ \AA}$ with cross-sectional diameter 20 \AA are considered; therefore $p = 25$ and χ can be assumed equal to unity. For these data at $kT = 4.14 \cdot 10^{-21}$ ($T = 300 \text{ K}$) the viscosity coefficients can be estimated from expressions (47):

$$a_1 = 2.203 \cdot 10^{-4} \text{ Pa}\cdot\text{sec}, \quad a_2 = a_3 = 7.399 \cdot 10^{-4} \text{ Pa}\cdot\text{sec}, \quad a_4 = 22.200 \cdot 10^{-4} \text{ Pa}\cdot\text{sec},$$

$$a_5 = 19.930 \cdot 10^{-4} \text{ Pa}\cdot\text{sec}, \quad a_6 = -28.910 \cdot 10^{-4} \text{ Pa}\cdot\text{sec}, \quad a_7 = 9.525 \cdot 10^{-4} \text{ Pa}\cdot\text{sec}, \quad a_8 = 28.97 \cdot 10^{-4} \text{ Pa}\cdot\text{sec}.$$

The viscosity coefficients a_i allow one to calculate the so-called Leslie coefficients:

$$\alpha_1 = a_8, \quad \alpha_2 = a_6 - a_5, \quad \alpha_3 = a_7 - a_6, \quad \alpha_4 = a_2 + a_3,$$

$$\alpha_5 = a_5 + a_6, \quad \alpha_6 = a_6 + a_7, \quad \gamma_1 = \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_2 + \alpha_3.$$

In order of magnitude, the viscosity coefficients are close to the shear-viscosity coefficient of water, which is a solvent containing fragments of a DNA molecule. The negative value of a_6 is due to the approximate character of expressions for the microscopic tensor of stresses and correlator of the tensor order parameter. It is essential that viscosity be an anisotropic characteristic of the medium.

NOTATION

B_{ijkl}^α ($\alpha = 1, 2, 3$), Stratanovich matrices (see, e.g., [2]); b , quantity characterizing the intensity of interaction of a selected molecule with its surroundings; \mathbf{c}_i^v , projection of a unit vector \mathbf{c}^v directed along the axis of the DNA molecule fragment numbered v onto the x_i axis; D , coefficient of rotational diffusion; e_{mlk} , Levi-Civita tensor; $F_i^{\nu\mu}$, i th projection of the force of interaction of two particles numbered v and μ ; k , Boltzmann constant; N , number of molecule fragments in the system; $n = N/V$, density of the number of fragments; n_i , director; $p = L_p/d$, ratio of the molecule length L_p to its diameter d ; p_i^v , projection of the pulse of a particle numbered v onto the x_i axis; s , scalar

ordering parameter of ordering; T , absolute temperature; t , time; U , single-particle potential energy of a molecule; V , volume of the system; X_j^{vu} , projection of the vector that connects the centers of mass of two particles on the x_j axis; \mathbf{x}^v , radius-vector of the center of mass of the fragment of the DNA molecule numbered v ; $\beta = (kT)^{-1}$; δ , form-factor, dimensionless quantity, depending on the ratio of L_p to d ; $\delta(\mathbf{x} - \mathbf{x}^v)$, Dirac delta function; δ_{ij} , Kronecker symbol; $\dot{\epsilon}_{kl}$, tensor of deformation rates; η , viscosity of the medium; ξ , coefficient of rotational friction; τ_α , relaxation time; ϑ_k , flow velocity of the medium; Ω , volume of the DNA molecule fragment the length of which is equal to its persistent length; ω_m , mean angular velocity of the proper rotation of the medium molecules. Subscripts: a, antisymmetric part; b, bases; p, persistent; s, symmetrical part; \wedge , microscopic value. Superscripts: over bar, average value; ', variables with respect to which integration is made.

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