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CONCENTRATION DEPENDENCES OF THE DYNAMIC PROPERTIES OF NaCl AQUEOUS SOLUTION ON THE BASIS OF THE RESULTS OF MOLECULAR DYNAMICS AND QUASI-ELASTIC NEUTRON SCATTERING RESEARCHES

The results of researches concerning the influence of the concentration on the structural and dynamic properties of a NaCl aqueous solution in the concentration interval $0.00 \leq X_{\mathrm{NaCl}} \leq 0.28$ *m.f. at the temperature* $T = 300$ *K obtained using the molecular dynamics and quasi-elastic neutron scattering methods are reported.*

Keywords: aqueous solution, electrolyte, molecular simulation, hydration shell, dwell time, diffusion coefficient.

1. Introduction

In recent years, a considerable contribution has been made to the development of the microscopic theories of fluid systems that allow one to satisfy the requirements of chemistry [1], biochemistry [2], and molecular biology [3]. On the one hand, water and ions are the inherent components of blocks used at the calculation of biomolecular systems. On the other hand, they are directly used to describe the properties of proteins, e.g., while describing the penetration of ions through membranes in aqueous solutions of proteins [4]. Therefore, the necessity in a correct description of their mutual interaction is undoubtful.

Information concerning the structural, thermodynamic, and dynamic properties of electrolyte solutions is highly important for the understanding and optimization of numerous processes, first of all, which are connected with reactions in electrochemical and biological fluid systems. The so-called biological fluids are often used today as an experimental model, while developing diagnostic techniques and creating new approaches that involve the specific features of examined alive systems [5]. The term “biological fluids” includes not only fluids in alive organisms (blood, lymph, extra- and intercellular fluids), but also artificial model ones. One of the latter is the aqueous solution of sodium chloride, which is widely used in medicine.

The correct description of the interaction in biological fluids demands a comprehension of processes at the molecular level. It can be done with the help of numerical simulations, in particular, with the use of the Monte Carlo or the molecular dynamics method. Taking into account that the influence of ions and their concentration on the processes of water structure formation is important for the understanding of the protein stability, the research of the properties of biological fluids, namely, those of the aqueous solution of sodium chloride, at various concentrations is important and challenging.

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2. Research Methods

2.1. Description of the model and the details of a computer experiment

In our researches, we selected a molecular model of fluid and a pair potential that is a sum of the Lennard-Jones and Coulomb components [6],

$$U = U_{\mathrm{LJ}} + U_{\mathrm{C}} = \sum_{ij} 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \\ + \sum_{ij} \frac{q_i q_j}{r_{ij}}, \qquad (1)$$

where the constants ε_{ij}, σ_{ij}, and q_i are obtained on the basis of model representations and the analysis of experimental data, and r_{ij} is the distance between interacting particles. The parameters ε_{ij} and σ_{ij} describing the interaction between the atoms of solvent and solute molecules are calculated with the help of the Lorentz–Berthelot combination rule [7]:

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}, \quad \varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}. \qquad (2)$$

The values used for the charges and the Lennard-Jones parameters σ and ε for water, anions, and cations [7], as well as their masses, are quoted in Table 1.

The influence of the electrolyte concentration on the energy, structure, and dynamic characteristics of the aqueous solution is studied using the molecular dynamics (MD) method. It is done with the help of the modified software package DLPOLY [8] with a time step of 2 fs and the periodic boundary conditions. The atoms of water molecules and ions were simulated as solid-like charged model systems with a fixed geometry. The parameters of intermolecular interaction were obtained on the basis of the atom-to-atom representation for the interaction between particles of various kinds with the use of the Lorentz–Berthelot rule. The elementary cell volume corresponds to the experimental density of a NaCl aqueous solution at $T = 300$ K. The atom-to-atom interactions with the participation of water molecules and ions are described with the help of the OPLS potentials for fluid systems [9]. The interaction between water molecules is described with the use of the SPC/E potentials [7]. The stabilization of the system in an NVT ensemble is performed, by applying a method proposed in work [9]. The electrostatic interaction between particles is taken into account, by using the Ewald summation [9]. The calculations are carried out according to the following scheme: the stabilization of the examined system is reached after 10^8 steps; then, 10^6 calculation steps are made. All radial distribution functions (RDFs) are obtained with a step of 200 fs. One of the leading places in researches with the help of numerical methods belongs to the calculation and analysis of RDFs, which characterize the probabilities of atomic arrangement in the system [6] and make it possible to determine the probability density to find the atoms of kind "y" around the atoms of kind "x" as a function of the distance between them:

$$G_{xy}(R) = \frac{\langle N_y\,(R, R + dR)\rangle}{\rho_y 4\pi R^2 dR}. \qquad (3)$$

The expression in the numerator equals the average number of "y" atoms in a spherical layer with the radius varying from R to $R + dR$, whereas the denominator normalizes the distribution so that $G_{xy} = 1$ at N_y and equals the density $\rho_y = N/V$. The integration of the RDF up to the first maximum allows the number of the nearest neighbors to be precisely determined. It should be noted that the position of the first RDF maximum is identified with the interatomic bond length, whereas the positions of the first and second minima of the RDFs are identified with the dimensions of the first and second hydration spheres, respectively. The first hydration sphere is defined as a space within a sphere, whose radius is equal to the position of the first RDF minimum. The second hydration sphere is defined as the space occupied by a spherical layer with its radius varying from the first RDF minimum to the second one.

Table 1. **Model parameters**

Atom	q, e	σ, A	ε, kcal/mol	M, u.
H	+0.41	1.0	0.15488	1.0
O	−0.82	3.166	0.65020	15.990
Cl^-	−1	4.75	0.1182	34.454
Na^+	+1	2.62	0.115661	22.9897

While analyzing the network of hydrogen bonds between water molecules, the following criterion is used: a hydrogen bond can be formed provided that the distance between the nearest oxygen atoms in a water molecule does not exceed 3.5 Å. As the hydrogen bond between the nearest neighbors, we select a bond with the distance between the O and H atoms that is minimal among all possible intermolecular distances. The hydrogen bond angle was defined as the angle between the O–H bond vector in one water molecule and the O–H bond vector in the other water molecule in the interval from 130° to 180° [10].

2.2. Quasi-elastic neutron scattering in the research of fluids

The dynamic properties of NaCl aqueous solutions with various concentrations were studied, by using the quasi-elastic neutron scattering (QENS) method [11]. This method is known to be highly sensitive to the dynamics of molecules in hydrogen-containing fluids. In addition, it makes it possible to monitor the molecular diffusion motions within time intervals from 10^{-12} to 10^{-10} s and, hence, to obtain information concerning the collective and one-particle motions of molecules. The time-of-flight spectra of quasi-elastic scattering of slow neutrons are measured on a WMR-M reactor equipped with a multidetector spectrometer at the Institute for Nuclear Research of the National Academy of Sciences of Ukraine (Kyiv).

In order to elucidate the role and share of the collective contribution to the formation of the self-diffusion coefficient of solvent molecules, we studied the scattering of slow neutrons in NaCl aqueous solutions with various concentrations of ions. The broadening of a quasi-elastic peak in those solutions was determined following a technique described in work [12]. Note that the dissolution of salts in water is accompanied by the hydration of ions. Some solvent molecules interact immediately with ions to form hydration shells around them. But the influence of ions on the fluid structure is not reduced to the short-range hydration only. The whole mass of water in a solution undergoes the influence of a strong electrostatic field created by ions. For a more detailed information on self-diffusion to be obtained, one should also know the influence of ions on the structure of water, whose molecules are not included into the hydration shells of ions, i.e. on the structure of the so-called free water. The complete dynamics of solvent molecules in ionic solutions consists of two components: collective and one-particle ones [13]. The rapid one-particle motions of free water molecules in the solution (the "Frenkel" diffusion mechanism) compose a one-particle contribution to the total self-diffusion coefficient. The role of a "Lagrange" particle in the solution is played by a hydrated ion that moves together with water molecules strongly bounded with it as a whole (the collective mechanism of diffusion). Hence, the water molecules can participate both in the one-particle motion between the hydration shells and in the collective motion together with their hydration shells. Proceeding from the time scale hierarchy of dynamic processes, the broadening of the quasi-elastic peak $\Delta E = \Delta E\,(Q)$ can be presented in the form

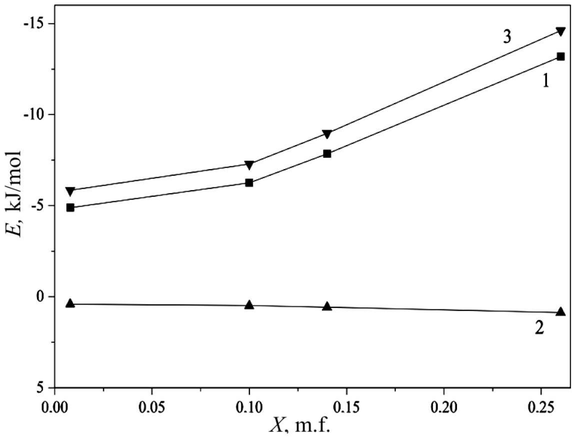


Fig. 1. Concentration dependences of the average total energy of intermolecular interaction $\langle E_{\rm sum}\rangle$ (curve *1*) and its van der Waals, $\langle E_{\rm VdW}\rangle$ (curve *2*), and Coulomb, $\langle E_{\rm C}\rangle$ (curve *3*), components in the NaCl aqueous solution at $T = 300$ K

$$\Delta E = \Delta E_{\rm K} + \Delta E_{\rm O}, \tag{4}$$

where $\Delta E_{\rm K}$ and $\Delta E_{\rm O}$ are the collective and one-particle, respectively, contributions to the quasi-elastic peak broadening. Using the equation for the experimentally observed broadening of quasi-elastic peak [14, 15],

$$\Delta E = 2\,\hbar\, D_{\rm K} Q^2 + \frac{2\hbar}{\tau_0}\left[1 - \frac{\exp\{-2W\}}{1 + Q^2 D_{\rm o}\tau_0}\right], \tag{5}$$

where τ_0 is the dwell time of a molecule at the equilibrium position, and $\exp\{-2W\}$ is the Debye–Waller factor, we can determine the collective, $D_{\rm k}$, and one-particle, $D_{\rm o}$, contributions to the self-diffusion coefficient $D = D_{\rm k} + D_{\rm o}$.

3. Results of Theoretical and Experimental Researches

3.1. Energy and structural properties of a NaCl aqueous solution

A computer experiment was carried out to obtain the energy and the structural and dynamic characteris-

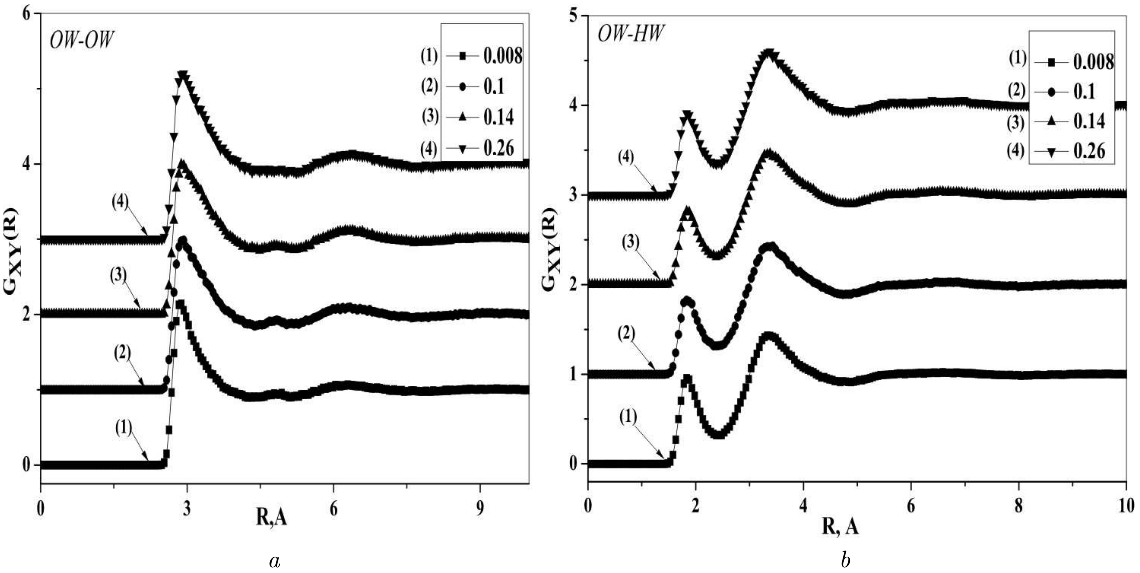


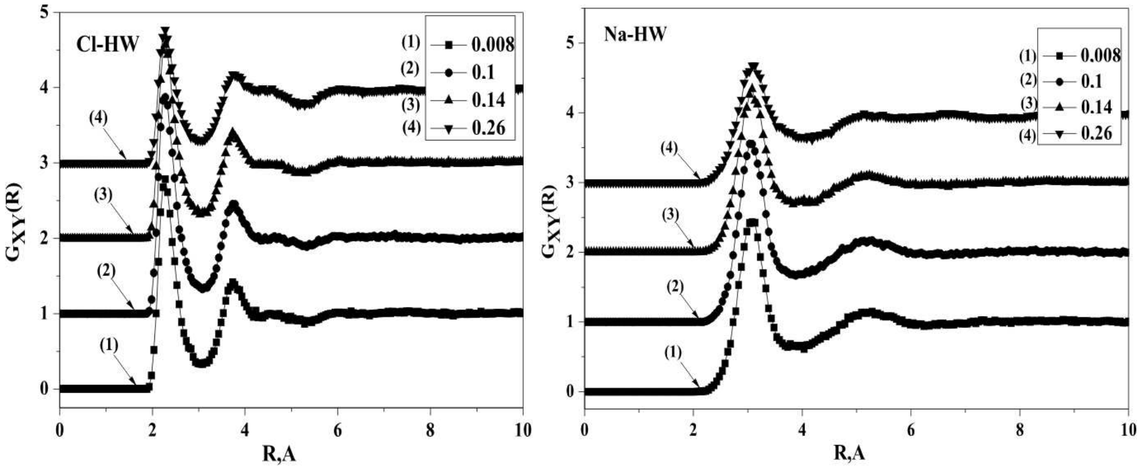
Fig. 2. RDFs $G_{XY}(R)^{\mathrm{OW-OW}}$ (*a*) and $G_{XY}(R)^{\mathrm{OW-HW}}$ (*b*) for various concentrations of NaCl–H_2O solution at $T = 300$ K

tics of a NaCl aqueous solution at $T = 300$ K. First of all, let us analyze the influence of the concentration on the average energy $\langle E_{\mathrm{sum}} \rangle$ of intermolecular interaction (Fig. 1) and its van der Waals, $\langle E_{\mathrm{VdW}} \rangle$, and Coulomb, $\langle E_{\mathrm{C}} \rangle$, components in the examined systems.

The data obtained demonstrate that the salt concentration growth gives rise to a reduction of both $\langle E_{\mathrm{sum}} \rangle$ and $\langle E_{\mathrm{C}} \rangle$, which testifies to an increase of the role of short-range interactions in the system and can diminish the mobility of its components. The analysis of the concentration dependences of $\langle E_{\mathrm{C}} \rangle$ and $\langle E_{\mathrm{sum}} \rangle$ shows that a reduction of the energy is not linear. This enables us to distinguish a number of concentration intervals: $X_{\mathrm{NaCl}} \leq 0.10$ m.f., 0.10 m.f. $\leq X_{\mathrm{NaCl}} \leq 0.14$ m.f., and 0.14 m.f. $\leq$ $\leq X_{\mathrm{NaCl}} \leq 0.28$ m.f.. It should be noted that in the intervals $X_{\mathrm{NaCl}} \leq 0.10$ m.f. and 0.10 m.f. $\leq$ $\leq X_{\mathrm{NaCl}} \leq 0.14$ m.f., the values of $\langle E_{\mathrm{sum}} \rangle$ and $\langle E_{\mathrm{C}} \rangle$ change considerably. At the same time, in the interval 0.14 m.f. $\leq X_{\mathrm{NaCl}} \leq 0.28$ m.f., the changes of both $\langle E_{\mathrm{sum}} \rangle$ and $\langle E_{\mathrm{C}} \rangle$ are insignificant, which testifies to a certain stability of the structure formation processes in the fluid. Hence, certain features in the local structure formation in the examined fluid systems should expectedly take place at concentrations in vicinities of $X_{\mathrm{NaCl}} \approx 0.10$ and 0.14 m.f., which should find their correspondence in the RDF behavior.

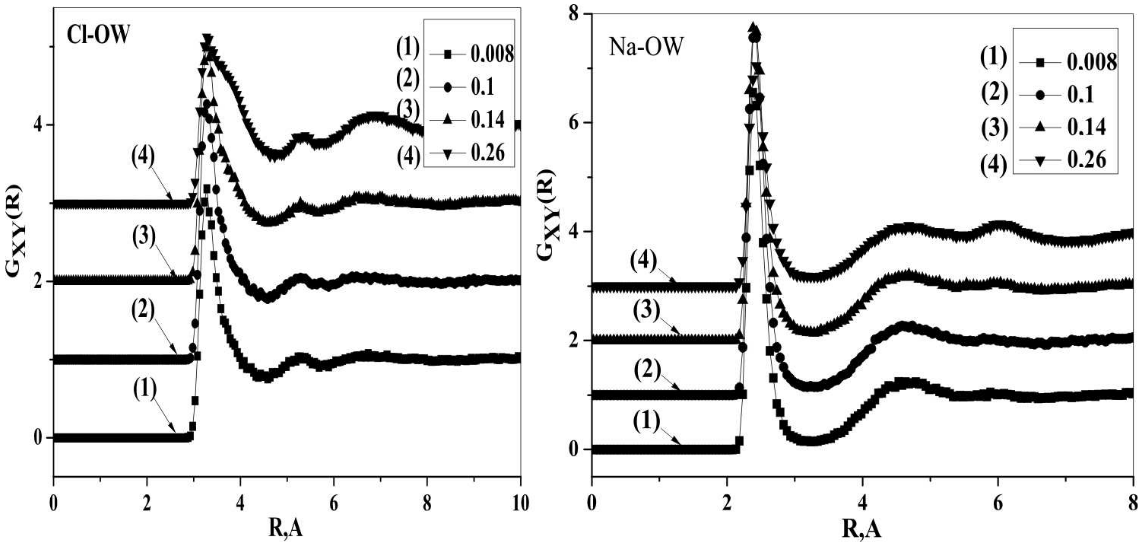
The determination of the features in the influence of the NaCl concentration on the processes of local structure formation in water is expedient to be started from the analysis of the concentration influence on the interaction between water molecules. In Fig. 2, the concentration dependence of the RDF, which characterizes the probability for water molecules to interact with each other, is presented. The increase of the RDF with the electrolyte concentration (Fig. 2, *a*) allows us to assert that, as the electrolyte content in the system grows, the probability for water molecules to interact with each other increases, keeping the distance between the interacting molecules constant (2.8 ± 0.1 Å). Starting from the concentration $X_{\mathrm{NaCl}} \approx 0.14$ m.f., an increase of the first hydration shell dimensions and a reduction of the RDF at the first minimum are observed, which testifies to the growth of the local density of the researched systems with the concentration. The invariance of the first maximum position in the RDF $G_{XY}(R)^{\mathrm{OW-HW}}$ (see Fig. 2, *b*) shows that the length of hydrogen bonds between water molecules does not change, as the salt concentration in the system grows.

The features in the influence of the salt concentration on the local structure formation in the water–NaCl systems can be deduced from the analysis of the RDFs (Figs. 3 and 4) describing the



a *b*

Fig. 3. The same as in Fig. 2, but for the RDFs $G_{XY}(R)^{\mathrm{Cl-HW}}$ (*a*) and $G_{XY}(R)^{\mathrm{Na-HW}}$ (*b*)



a *b*

Fig. 4. The same as in Fig. 2, but for the RDFs $G_{XY}(R)^{\mathrm{Cl-OW}}$ (*a*) and $G_{XY}(R)^{\mathrm{Na-OW}}$ (*b*)

probabilities of interactions $\mathrm{Na}^{+}...\mathrm{H}^{\mathrm{W}}$, $\mathrm{Cl}^{-}...\mathrm{H}^{\mathrm{W}}$, $\mathrm{Na}^{+}...\mathrm{O}^{\mathrm{W}}$, and $\mathrm{Cl}^{-}...\mathrm{O}^{\mathrm{W}}$. Of special interest is the interaction $\mathrm{Cl}^{-}...\mathrm{H}^{\mathrm{W}}$, which is responsible for the formation of stable hydrogen-bonded complexes $\mathrm{Cl}^{-}...\mathrm{H}^{\mathrm{W}}...\mathrm{O}^{\mathrm{W}}$ 2.3 Å in length, which is not affected by a change of the electrolyte concentration in the solution. The probability of such interactions increases with the electrolyte concentration in the system.

The RDF decreases with increasing the electrolyte content in the system, except for the concentration $X_{\mathrm{NaCl}} \approx 0.10$ m.f. The interaction between anions and cations makes the most substantial influence on the formation of a local structure in the solution, and its probability decreases with increasing the electrolyte concentration in the examined system, which is associated with a reduction in the number of free anions and cations. Up to four hydration shells can

Table 2. **Diffusion coefficient of water, its collective contribution, and the dwell time of molecules in NaCl–H$_2$O solutions with various concentrations**

Medium	Concentration X, m.f.	Diffusion coefficient of water $D \cdot 10^9$, m^2/s	Collective contribution to self-diffusion coefficient, $D_K \cdot 10^9$, m^2/s	$\frac{D_K}{D} \cdot 100\%$	Dwell time τ_o, 10^{-12} s
H$_2$O	–	2.30 ± 0.10	0.26 ± 0.04	11	1.73 ± 0.10
NaCl–H$_2$O	0.6	2.0 ± 0.10	0.27 ± 0.01	13.5	1.91 ± 0.05
	0.11	1.73 ± 0.09	0.32 ± 0.02	18	2.05 ± 0.05
	0.17	1.52 ± 0.10	0.33 ± 0.03	22	2.41 ± 0.04
	0.23	1.34 ± 0.08	0.35 ± 0.02	26	2.80 ± 0.03

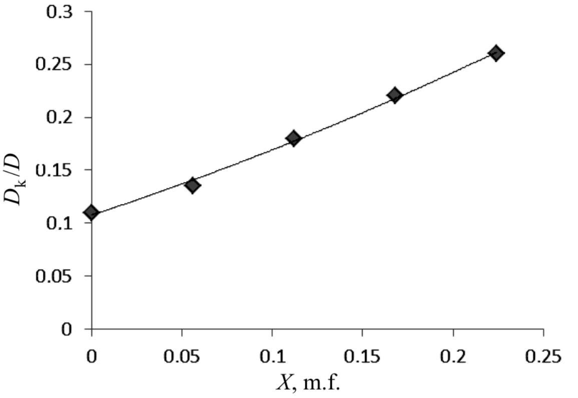


Fig. 5. Dependence of the relative magnitude of collective contribution to the diffusion coefficient of water on the concentration of a NaCl–H$_2$O solution

be formed around Cl$^-$ and Na$^+$ ions (see Figs. 3 and 4).

3.2. Dynamic properties of a NaCl aqueous solution according to QENS data

The results obtained in the neutron experiment for NaCl aqueous solutions with various concentrations are quoted in Table 2. It should be noted that the cross-section of scattering of slow neutrons by hydrogen atoms is approximately 20 times larger than those for other atoms. This fact results in that neutrons, when being scattered by water molecules, mainly "feel" the motions of hydrogen atoms and, consequently, provide information concerning the dynamics of water molecules only within the scope, within which this dynamics reveals itself in the motions of hydrogen atoms.

The dependence of the relative magnitude of collective contribution to the water diffusion coefficient on the NaCl–H$_2$O solution concentration is depicted in Fig. 5. For NaCl–H$_2$O solutions, the magnitude of collective contribution to the self-diffusion coefficient increases with the concentration, whereas the total self-diffusion coefficient decreases. This is associated, in our opinion, with the hydration effect. In this case, for the water molecules in hydration shells, their participation in the self-diffusion and in the exchange processes between free water molecules and molecules in neighbor hydration shells becomes complicated. Moreover, as the concentration grows, the number and the size of "Lagrange" particles increase as a result of the hydration, which increases the obstacle effect and gives rise to the growth of the collective contribution to the self-diffusion coefficient of water molecules.

Under the conditions of positive hydration, the neighbor water molecules spend more time, on the average, near an ion than in the coupling with one another. The corresponding dwell time of water molecules at the equilibrium position increases in comparison with the case of pure solvent. The determination of the composition of "Lagrange" particles and the estimation of the hydration effect influence on the self-diffusion processes in an aqueous solution of sodium chloride can be carried out by analyzing the number of nearest neighbors, which is proportional to the area under the first peak in the corresponding RDFs [6].

The analysis of the numbers of nearest neighbors N calculated in the case of concentrations $X_{\mathrm{NaCl}} <$ < 0.05 m.f. testifies that, in the solution, there are systems consisting of two or three water molecules. The obtained result correlates with the data of work [16]. According to the latter, the average energy of interaction between molecules in water composed by clusters consisting of three molecules amounts to 1.6 kcal/mol. According to the results of our calculations (Fig. 1), the total energy of the system at concentrations $X_{\mathrm{NaCl}} < 0.05$ m.f. equals $1.2 \pm \pm 0.5$ kcal/mol. In other words, we may assume that, at $X_{\mathrm{NaCl}} < 0.05$ m.f., ions and cations in the aqueous solution do not interact with one another, but only give rise to a break of the network of hydrogen bonds between water molecules. In turn, this process results in the formation of systems consisting of one, two, or three water molecules.

At concentrations 0.1 m.f. $\leq X_{\mathrm{NaCl}} \leq 0.2$ m.f., the growth in the number of Na^+ and Cl^- leads to the formation of ion-cation pairs. Simultaneously, free Na^+ and Cl^- ions surrounded by water molecules continue to exist in the solution. This means that all those systems (free Na^+ and Cl^- ions, and ion-cation groups surrounded by water molecules) are "Lagrange" particles. The growth of the electrolyte content in the concentration interval 0.1 m.f. $\leq X_{\mathrm{NaCl}} \leq 0.2$ m.f. is accompanied by a reduction of the self-diffusion coefficient, which is associated with the formation of relatively large systems owing to the interaction of ions with water or with one another.

Starting from the concentration $X_{\mathrm{NaCl}} \approx 0.2$ m.f., the overwhelming majority of ions can be considered as interacting with one another. At $X_{\mathrm{NaCl}} \approx \approx 0.24$ m.f., owing to this interaction, rather large systems composed of $N_z = (16 \pm 0.3)$ particles are formed. At the same time, e.g., in a vicinity of $X_{\mathrm{NaCl}} \approx 0.24$ m.f., there exist systems consisting of a Na^+ ion surrounded by $N_z = (6 \pm 0.3)$ water molecules, or a Cl^- anion surrounded by $N_z = (4 \pm 0.3)$ water molecules, or clusters of water molecules. In the concentration interval near $X_{\mathrm{NaCl}} \approx 0.24$ m.f., the water clusters include three molecules. This fact testifies to the stabilization of local ionic and water-ionic structures in the saturated water-salt solution and to the existence of a water structure similar to "pure" water.

4. Conclusions

The application of experimental (quasi-elastic neutron scattering) and theoretical (molecular simulation) methods for studying the concentration features in NaCl aqueous solutions allowed us to determine the structural and dynamic properties of a NaCl aqueous solution at $T = 300$ K. It is found that, at concentrations $X_{\mathrm{NaCl}} \leq 0.05$ m.f., the motion of Na^+ and Cl^- ions, noninteracting with one another, results in the break of the network of hydrogen bonds between water molecules and in the formation of systems composed of one to three water molecules. In the concentration interval 0.05 m.f. $\leq X_{\mathrm{NaCl}} \leq 0.1$ m.f., ion-cation pairs are formed, as well as systems of Na^+ and Cl^- ions composed of $N_z = (7 \pm 0.3)$ particles. At 0.1 m.f. $\leq X_{\mathrm{NaCl}} \leq 0.2$ m.f., the self-diffusion coefficient of ions decreases, which is associated with the formation of large systems owing to the interaction of ions with water and with one another. At $X_{\mathrm{NaCl}} \approx 0.2$ m.f., most of Na^+ and Cl^- ions interact with one another. In the saturated solution at $X_{\mathrm{NaCl}} \approx 0.26$ m.f., Na^+ and Cl^- ions form systems of $N_z = (16 \pm 0.3)$ particles.

The results of calculations quantitatively supplement the experimental QENS data, according to which a monotonic reduction of the self-diffusion coefficient, its components, and the dwell time of molecules in the equilibrium state is observed in the examined system, as the NaCl concentration in water increases. The growth of the collective contribution to the self-diffusion coefficient testifies to the presence of vibration centers in the solution, the role of which is played by Na^+ and Cl^- ions surrounded by hydration shells. According to the data of MD calculations, in the case of the interaction between ions and water molecules, the number of hydration shells reaches a value of four.

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КОНЦЕНТРАЦІЙНІ ЗАЛЕЖНОСТІ ВЛАСТИВОСТЕЙ ВОДНОГО РОЗЧИНУ ХЛОРИДУ НАТРІЮ ПО ДАНИХ МЕТОДІВ МОЛЕКУЛЯРНОЇ ДИНАМІКИ ТА КВАЗІПРУЖНЬОГО РОЗСІЮВАННЯ НЕЙТРОНІВ

Резюме

В роботі представлено результати досліджень впливу концентрації однозарядного електроліту на енергетичні, структурні та динамічні властивості водного розчину NaCl при $T = 300$ K за концентрацій $0,00 \leq X_{\mathrm{NaCl}} \leq 0,28$ м.д. методами молекулярної динаміки та квазіпружного розсіяння нейтронів.