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Spectral Effects of the Clusterization of Greenhouse Gases: Computer Experiment

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Abstract—Autocorrelation functions of the total dipole moment of clusters composed of H_2O and N_2O molecules are calculated in terms of the molecular dynamics method. The IR absorption and reflection spectra of systems composed of $(H_2O)_i$, $N_2O(H_2O)_i$, and $(N_2O)_2(H_2O)_i$ clusters ($2 \le i \le 20$) are obtained on the basis of these functions. Frequency-dependent dielectric permittivity of clusters increases after the absorption of N_2O molecules. The absorption coefficient of cluster systems with trapped N_2O molecules increases at low frequencies and decays at frequencies $\omega > 500$ cm^{-1}. The inclusion of N_2O molecules increases also reflection coefficient R and changes the pattern of $R(\omega)$ spectra. The absorption of IR radiation increases with the number of H_2O molecules in clusters. Dielectric losses also increase with an increase in i number upon the absorption of N_2O molecules. The number of electrons interacting with an incident electromagnetic wave increases upon the capture of N_2O molecules.

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INTRODUCTION

Dielectric relaxation provides information on the processes of the reorientation of polar molecules in the condensed media. Molecular processes responsible for the dielectric relaxation are described by the time correlation function of the total electric dipole moment. The study of such processes is of significant interest for the elucidation of the mechanism of cooperative dynamics of molecules, as well as for the interpretation of dielectric spectra [1]. In theoretical approaches, the diffusion limit or Debye's behavior are often considered; correlation functions of this behavior decay exponentially and can be described on the basis of only one relaxation time. However, in systems with hydrogen bonds, strong correlations of dipole moments are exhibited, thus making the Debye approximation impracticable. In this case, it is feasible to employ the computer simulation that correctly takes into account correlations of any type.

Quantum-chemical calculations for aqueous systems demonstrated the importance of the account of nonadditive contributions [2]. Three-particle interactions are responsible for about 10% of the total interaction energy of water trimer. In the case of solutions, many-particle forces can introduce still larger contribution. The effect of polarization in the water bulk is almost isotropic. One of the most encountered methods of the inclusion of nonadditive effects into the model is the account of polarization. Induced dipole moments of molecules depend on each other nonlinearly. The polarizability in the model of water can be attributed to single atoms emphasizing their ability to the dissociation and formation of ions. However, at not so close approach of two polarizable point elements, the value of polarizability increases infinitely. This event was called "polarization catastrophe" [3]. For real molecules, such a nonphysical event cannot take place. The use of decaying electric fields made it possible to lower the probability of polarization catastrophe. When the polarizability is attributed to the molecule as a whole, this divergence is not manifested and we can refuse the introduction of decay function.

Theoretical and experimental determination of IR spectra and the structure of water clusters presents a hard task. As the cluster size rises, the number of their isomers rapidly increases. There is a diversity of architectures of hydrogen atoms even for the determined size of cluster with a specific structural network of oxygen atoms. For example, only for the network of oxygen atoms arranged in the form of dodecahedron, the $(H_2O)_{20}$ cluster is characterized by about 30026 isomers differing in hydrogen bonds [4].

Computer simulation with empirical potentials gives correct coordination numbers and reasonable cation–oxygen distance $r_{\text{cat–O}}$. It is not the case for ab initio pair potentials that result in too large coordination numbers and distances $r_{\text{cat–O}}$ [5]. Calculations performed on the basis of ab initio principles are also characterized by overestimated values of vibration frequencies due to the neglect of many-particle forces.

The goal of this paper is to study the effect of the absorption of polar nitrogen oxide molecules by water clusters on the basis of the molecular dynamics method using the empirical potential and allowing for the polarizability of molecules. In this work, we focused our attention on the absorption and IR reflection spectra of aqueous disperse systems and estimated the effect of N_2O molecules attached to clusters on the rate of stored dissipation energy and the number of electrons participating in the interaction between aggregates and IR radiation. Water vapor and nitrogen oxide are greenhouse gases. Moreover, water vapor contributes mainly (to 95%) to Earth's greenhouse effect. The share of N_2O in the greenhouse effect is not so large (≈0.95%); however, the lifetime of N_2O in the atmosphere is comparable with that of carbon dioxide (the contribution to greenhouse effect is 3.62%) and considerably exceeds corresponding characteristics for methane (0.36%) and fluorocarbons (0.072%) [6]. In this work, in contrast to [7], we consider not only the effect of the absorption of N_2O molecules on spectral characteristics of water clusters but also analyze the growth of heteroclusters owing to the addition of water molecules.

COMPUTER MODEL

We used improved TIP4P potential [8] and rigid four-center model of water molecule. The geometry of monomer in this model is constructed on the basis of the study of the gaseous phase of water: the length of O–H bond is assumed as equal to 0.9572 Å and the H–O–H angle is 104.5°. Fixed charges are assigned to hydrogen atoms and point M lying on the bisectrix of H–O–H angle at a distance of 0.215 Å from the oxygen atom. The values of charges ($q_H = 0.519\ e$, $q_M = -1.038\ e$, e is the value of unit charge) and the position of point M were chosen such as to reproduce both the experimental values of dipole and quadrupole moments [9, 10], as well as the calculated ab initio energy of a dimer and characteristic distances in the dimer [11]. The model suggests the calculation of induced dipole moments of molecules that allows us to introduce the effect of their polarization into consideration. The description of interaction between N_2O molecules and water was based on atom–atom potentials calculated in the Gordon–Kim approximation using spherical averaging of electron densities [12, 13]. The N_2O molecule has the linear shape and is represented by three-center model with parameters $r_{ON} = 0.186$ nm [14], $q_{N_1} = 0.279\ e$, $q_{N_2} = -0.065\ e$, $q_O = -0.213\ e$ [13]. Note that the N_2O molecule is asymmetric relative to electric charges located in the positions of nitrogen atoms: one of these charges is positive and the other charge is characterized by small negative value. The H_2O and N_2O molecules possess permanent dipole moments and polarizabilities equal 1.848 D and 1.444 Å^3 and 0.396 D and 3.1 Å^3 [14], respectively.

First of all, we performed molecular dynamics calculation for water clusters with the number of molecules $2 \le i \le 20$. The final configuration of $(H_2O)_i$ clusters was hereafter used as the initial one for the simulation of heteroclusters. In the initial state, added molecules were located so that minimal distance between the atoms of impurity and water molecules composing the cluster would be no less than 0.6 nm. The cut-off radius of all interactions in a system was 0.9 nm. In the case of $(N_2O)_j(H_2O)_i$ ($j = 1, 2$) systems, added linear N_2O molecules were located along the rays connecting the center of mass of $(H_2O)_i$ clusters with the centers of mass of these molecules. The N_2O molecules were beyond the $(H_2O)_i$ cluster.

To integrate the equations of motion of the centers of molecule masses, we employed the forth-order Gear method [15]. The analytical solution of equations of the rotation of molecules was performed using the Rodrigues–Hamilton parameters [16]; the integration scheme of the equations of motion with rotations corresponded to the approach proposed by Sonnenschein [17]. Cluster temperature was constant (233 K) in the course of all calculations; the duration of calculation for each cluster was no less than $3 \times 10^6\ \Delta t$, where the time scale $\Delta t = 10^{-17}$ s. Calculations were performed using a PENTIUM-IV computer with processor clock frequency of 1.8 GHz. About 15 h of computation time was spent for the calculation (during time $10^6\ \Delta t$) of a cluster composed of 20 molecules.

In order to establish the effect of absorbed nitrogen oxide on the greenhouse effect, we consider ultradisperse systems of three types: (i) the region filled with water clusters composed of 2 to 20 molecules; (ii) the medium composed of $N_2O(H_2O)_i$ ($2 \le i \le 20$) clusters, where each cluster absorbed one N_2O molecule; and (iii) the set of $(N_2O)_2(H_2O)_i$, $2 \le i \le 20$ clusters, where each cluster absorbed two N_2O molecules.

In the order of sequence, we designate these systems by numbers I, II, and III.

DIELECTRIC PROPERTIES

Let us consider the case of scattering of unpolarized light on clusters, when mean free path l of molecules is much smaller than wavelength λ. The coefficient of extinction (attenuation), h, of incident beam is determined, on the one hand, by the Rayleigh formula [18] and, on the other hand, via the scattering coefficient ρ ($h = \frac{16\pi}{3}\rho$) [19] in the approximation of scattering at an angle of 90°. Assuming that $h = \alpha + \rho$, where α is the absorption coefficient, we have

$$N = \frac{2\omega^4}{3\pi c^4}\frac{(\sqrt{\varepsilon}-1)^2}{\alpha}\left(1-\frac{3}{16\pi}\right), \qquad (1)$$

where N is the number of scattering centers in 1 cm^3. Here, c is the speed of light, ε is the dielectric permittivity of a medium, and ω is the frequency of the incident wave.

Let us form systems I, II, and III from $(H_2O)_i$, $N_2O(H_2O)_i$, and $(N_2O)_2(H_2O)_i$ clusters, respectively, so that the cluster containing j molecules of impurity and i molecules of water has the statistical weight

$$W_{ij} = \frac{N_{ij}}{N_\Sigma}, \quad 2 \le i \le 20, \quad 0 \le j \le 2, \tag{2}$$

where N_{ji} is the number of clusters with i molecules of water and j molecules of nitrogen oxide in 1 cm^3, $N_\Sigma = \sum\limits_{i=2}^{20} N_{ij}$. Hereafter, the calculation of all spectral characteristics was performed with allowance for accepted statistical weights W_{ij}.

Static dielectric constant ε_0 was calculated via the fluctuations of total dipole moment **M** [20]

$$\varepsilon_0 = 1 + \frac{2\pi}{3VkT}[\langle \mathbf{M}^2 \rangle - \langle \mathbf{M} \rangle^2]. \tag{3}$$

Here, the total dipole moment of a cluster was calculated according to expression

$$\mathbf{M}(t) = Z_+ \sum_{i-1}^{N_1} \mathbf{r}_i(t) + Z_- \sum_{j=1}^{N_2} \mathbf{r}_j(t), \tag{4}$$

where $\mathbf{r}(t)$ is the vector indicating the position of atom i at moment t; Z is the electric charge located in the center of atom; and N_1 and N_2 are the numbers of atoms in the cluster carrying positive or negative charge, respectively. Index "+" refers to hydrogen or positively charged nitrogen; index "–", to oxygen or nitrogen carrying negative charge.

Dielectric permittivity $\varepsilon(\omega)$ was represented by complex value $\varepsilon(\omega) = \varepsilon'(\omega) - i\varepsilon''(\omega)$. To determine this value, we used the equation [20, 21]

$$\begin{aligned} \frac{\varepsilon(\omega) - 1}{\varepsilon_0 - 1} &= -\int_0^\infty \exp(-i\omega t)\frac{dF}{dt}dt \\ &= 1 - i\omega\int_0^\infty \exp(-i\omega t)F(t)dt, \end{aligned} \tag{5}$$

where function $F(t)$ reflects the normalized autocorrelation function of the total dipole moment of a cluster

$$F(t) = \frac{\langle \mathbf{M}(t) \cdot \mathbf{M}(0) \rangle}{\langle \mathbf{M}^2 \rangle}. \tag{6}$$

Frequency dispersion of dielectric permittivity determines the frequency dependence of dielectric losses, $P(\omega)$, in accordance with the expression [19]

$$P = \frac{\varepsilon' \langle E^2 \rangle \omega}{4\pi} \tan\delta, \tag{7}$$

where $\langle E^2 \rangle$ is the average value of the square of electric field strength and $\tan\delta = \varepsilon'/\varepsilon''$ is the dielectric loss tangent.

The absorption of electromagnetic waves of certain frequency by a molecule can occur only in the case when the dipole moment of a molecule oscillates with the same frequency. The absorption coefficient is proportional to the square of the oscillation amplitude of the dipole moment. The absorption of radiation at frequency ω at thermodynamic equilibrium in the gaseous phase with temperature T is characterized by absorption coefficient α. The α value can be represented via the imaginary part of frequency-dependent dielectric permittivity $\varepsilon(\omega)$ in the form [21]

$$a(\omega) = 2\frac{\omega}{c}\mathrm{Im}[\varepsilon(\omega)^{1/2}]. \tag{8}$$

Reflection coefficient R is defined as the ratio between the average energy flux reflected from the surface and the incident flux. Upon the normal incidence of plane monochromatic wave, the reflection coefficient is set by the formula [18]

$$R = \left| \frac{\sqrt{|\varepsilon_1|} - \sqrt{|\varepsilon_2|}}{\sqrt{|\varepsilon_1|} + \sqrt{|\varepsilon_2|}} \right|^2. \tag{9}$$

Here, it is suggested that the wave is incident from the transparent medium (medium 1) to the medium which can be both transparent and nontransparent, i.e., absorbing and scattering (medium 2). Indices at the dielectric permittivity in expression (9) denote the medium.

The total number of electrons, N_e, in unit cluster volume interacting with the external electromagnetic wave is set as [18]

$$N_e = \frac{m}{2\pi^2 e^2}\int_0^\infty \omega\varepsilon''(\omega)d\omega, \tag{10}$$

where m is the electron mass.

RESULTS OF CALCULATIONS

Configurations of $N_2O(H_2O)_{16}$, and $(N_2O)_2(H_2O)_{16}$ clusters at the instant 20 ps are represented in Fig. 1. In both cases, the N_2O molecule is brought into close contact with one of water molecules. At the same time, the stable bond is established between the N_2O molecules in the $(N_2O)_2(H_2O)_{16}$ cluster. The perturbation introduced by the addition of one N_2O molecule to the cluster is characterized as rather strong. In this case, one of the water molecules tends to leave the cluster. However, the immediate absorption of two closely located N_2O molecules leads to the rearrangement of the whole water cluster, thus making its shape more sphere-like.

System II composed of water clusters absorbed one N_2O molecule each has the largest values of both the real and imaginary parts of dielectric permittivity of a medium out of all systems considered (Fig. 2). The absorption of the second N_2O molecule by clusters

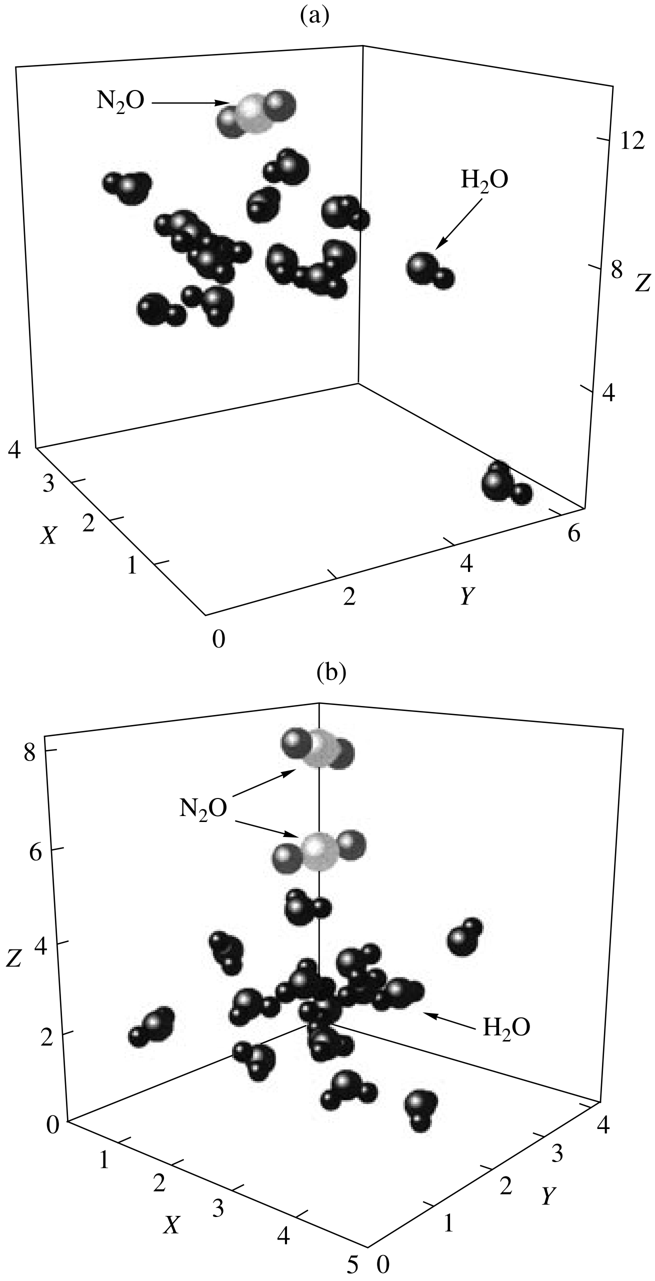

Fig. 1. Configurations of (a) $N_2O(H_2O)_{16}$ and (b) $(N_2O)_2(H_2O)_{16}$ clusters corresponding to time of 20 ps.

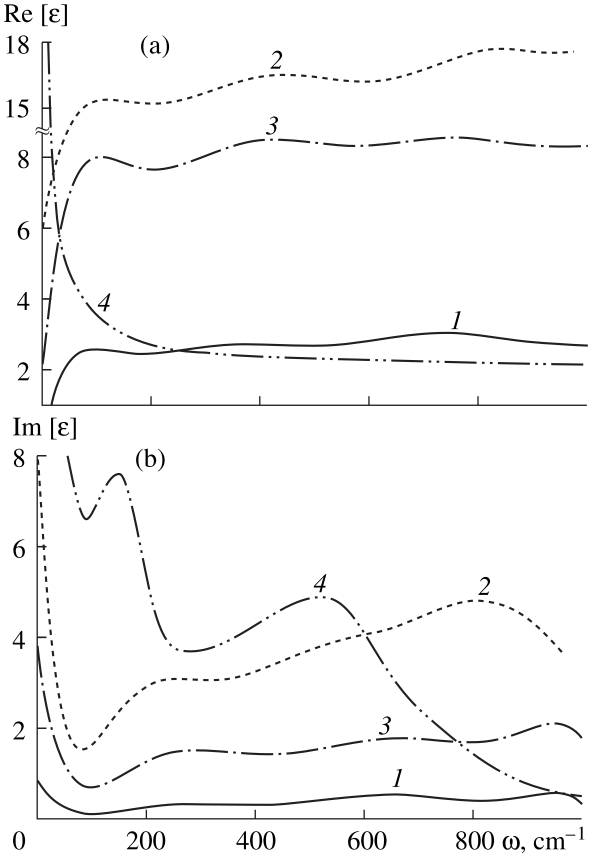

Fig. 2. Frequency dependences of (a) real and (b) imaginary parts of dielectric permittivity of cluster systems ($2 \leq i \leq 20$) (*1*) I, (*2*) II, and (*3*) III, and (*4*) bulk water: (a) [22] and (b) [23].

leads to some decrease in the ε' and ε'' values characterizing system III with respect to corresponding values for system II. System I composed of pure water clusters is characterized by the lowest ε' and ε'' values. The ε' values for systems II and III at frequencies higher than 30 cm^{-1} and for system I at frequencies higher than 245 cm^{-1} (Fig. 2a) are larger than corresponding value for the bulk water [22]. As is seen from this figure, the real part of dielectric permittivity, beginning with frequency $\omega \approx 100$ cm^{-1}, is noticeably less sensitive to the frequency than to the addition of N_2O molecules to clusters. The ε'' value for systems II and III is larger than experimental value ε'' for the bulk water [23] within the frequency range from 605 to 773 cm^{-1}; for system I, at $\omega > 960$ cm^{-1} (Fig. 2b). The change in the imaginary part of ε with frequency $\omega > 100$ cm^{-1} is comparable with the changes of this values caused by the addition of N_2O molecules to the clusters.

Clusters that absorbed the energy of IR radiation are transformed into the excited state and are capable of scattering the consumed energy. Frequency distribution of power *P* of the radiation emitted by cluster systems is shown in Fig. 3a. It is seen that, for each system, the *P* value rises with frequency. The *P*(ω) function changes considerably while passing from the system of pure water clusters (system I) to cluster systems containing one (system II) or two (system III) N_2O molecules. As a rule, the intensity of emission by clusters absorbing one N_2O molecule is by the order of magnitude higher. However, the absorption of the second N_2O molecule by the clusters decreases the power of their emission. System I dissipates the energy to a maximum extent at frequency of 973 cm^{-1}, whereas, for systems II and III, maximal frequencies decrease to 784 and 847 cm^{-1}, respectively. Dielectric loss tangent of these

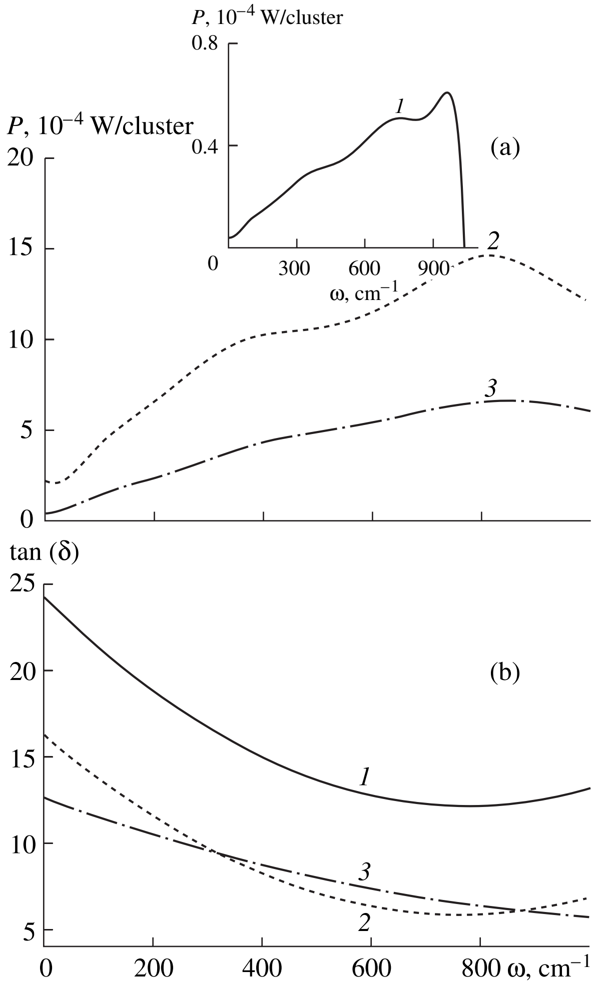

Fig. 3. Frequency dependences of (a) dielectric losses and (b) tangent of dielectric losses for systems (*1*) I, (*2*) II, and (*3*) III.

systems monotonically decreases with an increase in ω at the $\omega < 780\ \text{cm}^{-1}$ (Fig. 3b) passing through the minimum for systems I and II. For systems I and II, the extremum is determined by frequency $\omega = 784\ \text{cm}^{-1}$. Within the studied frequency range, the maxima of $\tan\delta(\omega)$ function are not observed for system III.

Spectral properties of cluster systems classified by the number of N_2O molecules in corresponding clusters are determined mainly by the physical properties of water molecule. Because the number of water molecules in systems I, II, and III is the same, the absorption spectra α(ω) of the IR radiation for these systems appeared also to be similar (Fig. 4). Compared to system I composed of pure water clusters, systems II and III containing N_2O molecules are featured by the larger probability of thermal absorption at the lowest frequencies ($\omega \le 550\ \text{cm}^{-1}$) and lower values of absorption coefficient α at frequencies $\omega > 600\ \text{cm}^{-1}$. Moreover, system III having the double amount of N_2O molecules than system II is characterized by larger values of coefficient α throughout the $0 \le \omega \le 1000\ \text{cm}^{-1}$ frequency range. Maximum values of absorption coefficient α(ω) of IR radiation for systems I, II, and III fall on frequencies 973, 910, and 847 cm^{-1}, respectively. Figure 4 shows also the α(ω) spectrum for real water [24]. Experimental α(ω) function for the bulk water has two maxima: the principal maximum corresponds to the frequency $\omega_\alpha = 700\ \text{cm}^{-1}$; the low-frequency maximum falls on 200 cm^{-1}. Coefficient α varies nonmonotonically with an increase in cluster size due to the addition of water molecule even when the number of H_2O molecules in the clusters varies from 10 to 20 (Fig. 5). The addition of second molecule can noticeably change the α(ω) spectrum of a single cluster. As a rule, clusters containing two N_2O molecules have larger number of peaks in the α(ω) spectrum. When passing from one to two N_2O molecules, integral intensity α of spectra, particularly for clusters containing 17 water molecules, also changes.

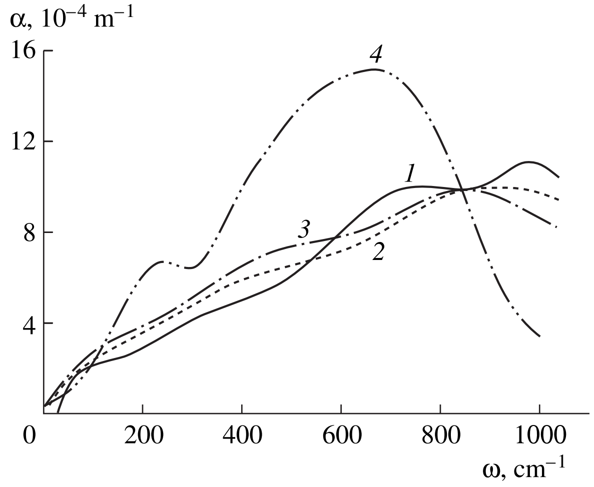

Fig. 4. Frequency dependences of absorption coefficient α of IR radiation by cluster systems (*1*) I, (*2*) II, and (*3*) III, and (*4*) bulk water [24].

After the addition of N_2O molecules to water clusters, reflection coefficient *R* of monochromatic electromagnetic wave by the disperse systems changes considerably (Fig. 6). First of all, this concerns an increase in the number of peaks in the *R*(ω) spectrum from five (for system I) to ten (for systems II and III). In the *R*(ω) spectrum for system I, peaks are separated by an interval of ≈200 cm^{-1}; in analogous spectra for systems II and III, the value of this interval decreases to ≈100 cm^{-1}. In other words, the addition of N_2O molecules to water clusters leads to the splitting of each peak of *R*(ω) spectrum into two peaks. In the $0 \le \omega \le 1000\ \text{cm}^{-1}$ frequency range, the reflection coefficient for system I varies from 0.022 to 0.042, i.e., the systems reflects only 2–4% of the energy of monochromatic electromagnetic wave. System II composed of clusters absorbed only one N_2O molecule each is characterized by the reflection coefficient that is by

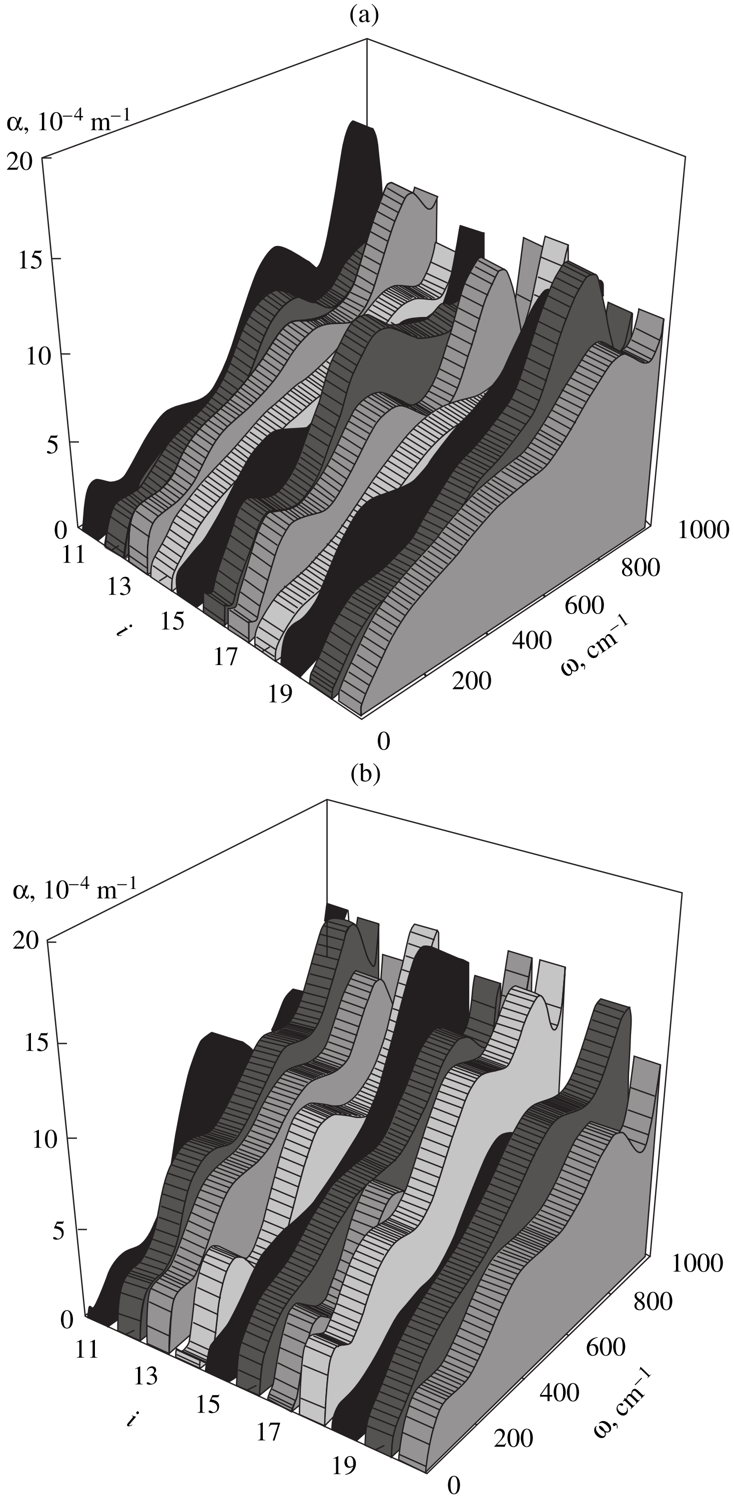

Fig. 5. The IR absorption spectra of (a) $N_2O(H_2O)_i$ and (b) $(N_2O)_2(H_2O)_i$ clusters.

almost one order of magnitude larger, i.e., this system reflects from 29 to 39% of the energy of IR radiation. The doubling of the number of N_2O molecules in a system, i.e., the passage to system III, does not increase but, on the contrary, decrease the reflection coefficient. In this case, the *R* value varies from 0.18 to 0.27. In general, for systems II and III, the reflection of electromagnetic wave asymptotically rises with increasing frequency; for system III, this parameter also increases but only to frequency of 580 cm^{-1}

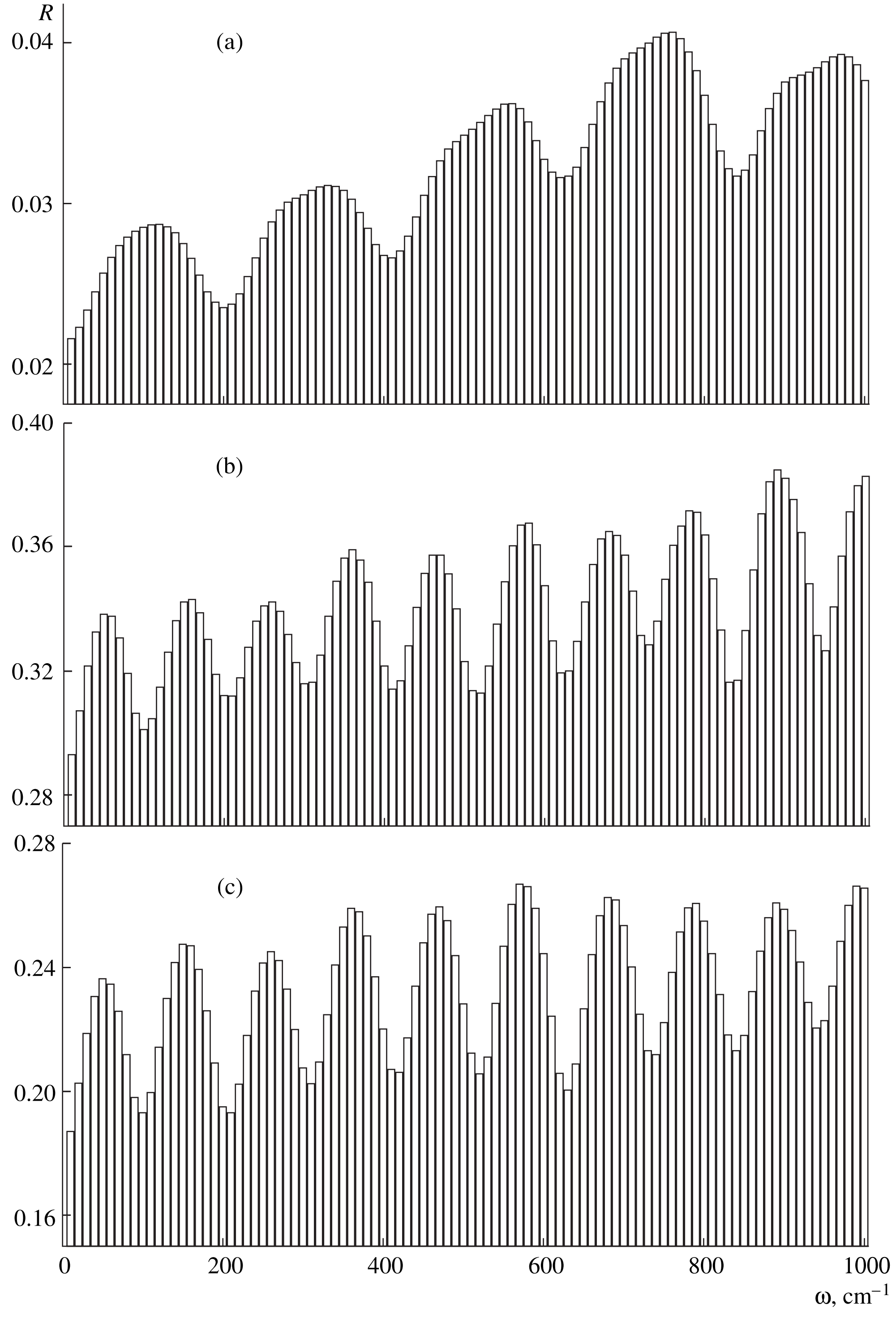

Fig. 6. Frequency dependences of the coefficient of reflection of plane monochromatic electromagnetic wave by disperse systems (a) I, (b) II, and (c) III.

and is not changed further. Upon the addition of water molecules to $N_2O(H_2O)_i$ and $(N_2O)_2(H_2O)_i$ clusters containing at least 10 H_2O molecules, coefficient R changes nonmonotonically (Fig. 7). The $N_2O(H_2O)_i$ clusters with $i = 12$ and 20 are characterized by the largest R values; cluster with $i = 13$, by the lowest R values. The $(N_2O)_2(H_2O)_i$ clusters have the largest R values at $i = 12$ and 15, whereas the cluster with $i = 18$ has the lowest R value. The value of the reflection coefficient is determined mainly by the cluster size

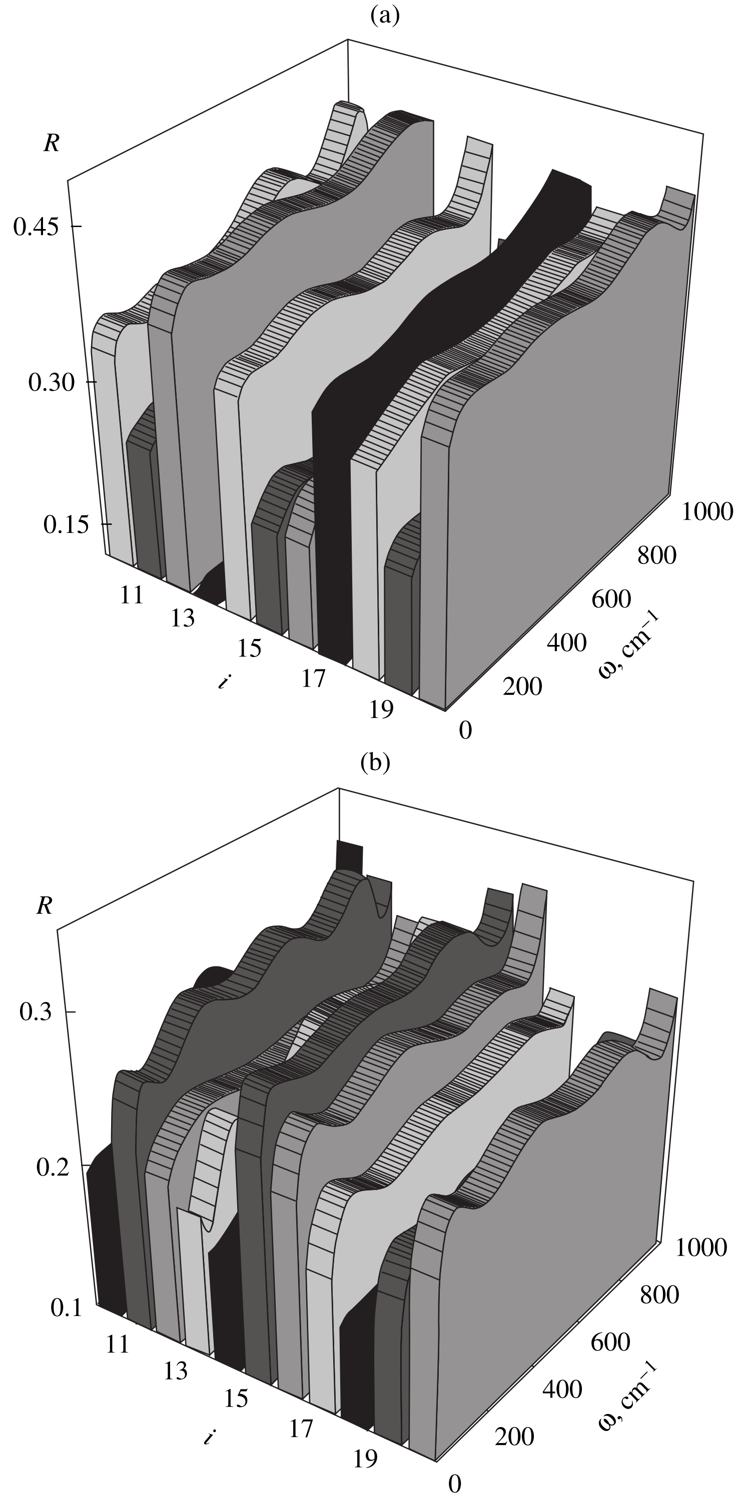

Fig. 7. The IR reflection spectra of (a) $N_2O(H_2O)_i$ and (b) $(N_2O)_2(H_2O)_i$ clusters.

rather than by the frequency. The addition of N_2O molecules drastically increases the diversity of cluster structures that, in general, leads to the doubling of the number of peaks. On the contrary, clusters of pure water are characterized by weaker dependence of R value on the aggregate size and stronger $R(\omega)$ dependence for each cluster.

Dependences of concentration n_e, the number of electrons that respond to incident IR radiation, on the

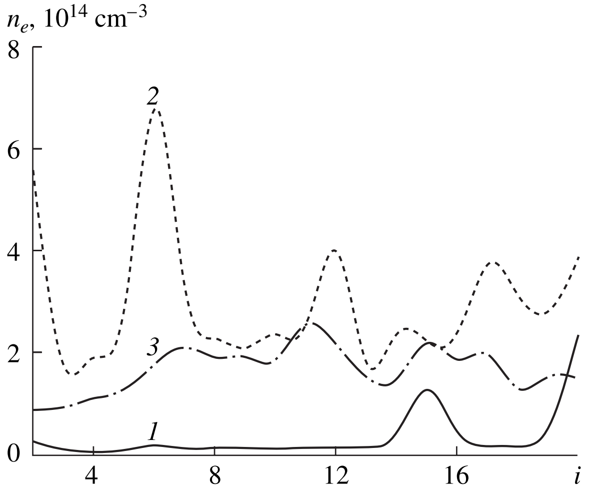

Fig. 8. The dependences of the density of electrons interacting with IR radiation on the size of (*1*) $(H_2O)_i$, (*2*) $N_2O(H_2O)_i$, and (*3*) $(N_2O)_2(H_2O)_i$ clusters.

cluster size are shown in Fig. 8. The $n_e(i)$ dependences for water clusters with sizes of $2 \le i \le 20$ are characterized by the peaks at $i = 15$ and 20. The number of electrons in clusters participating in the interaction with external electromagnetic radiation increases after the capture of N_2O molecules by the clusters. Moreover, this effect is most pronounced for clusters absorbing one N_2O molecule. Density peaks of n_e for these clusters are observed at $i = 2$, 5, 12, 14, 17, and 20; for $(N_2O)_2(H_2O)_i$ clusters, the major peak of $n_e(i)$ function falls on $i = 11$.

CONCLUSIONS

A large number of empirical potentials are used to describe the properties of pure water. On the basis of these potentials, phenomena observed in water are often better described with the molecular dynamics method than with more rigorous molecular-dynamics calculations that apply ab initio potentials. However, in some research fields such as wetting chemistry, biochemistry, and geochemistry, it is necessary to be particularly flexible in constructing potentials that account also for the charge transfer [25]. The ab initio calculation method is most suitable for describing these processes. It was demonstrated in this work that, within the framework of empirical force fields, hydrophilic interaction between the molecules of nitrogen oxide and water can be successfully studied. The absorption of N_2O molecules by the aqueous system leads to a significant rise of ε' and ε'' values. Moreover, the addition of second N_2O molecule to clusters makes the frequency dependence of these values stronger. After the addition of one N_2O molecule to the cluster, the rate of dissipation of accumulated energy considerably increases. The absorption of second N_2O molecule decreases the power of cluster emission. The value of $\tan\delta(\omega)$ strongly depends on the presence of N_2O molecules in a cluster. The absorption of N_2O molecules by water clusters results in a negligible change in the IR absorption spectra for systems studied. The cluster systems not only selectively dissipate incident electromagnetic radiation but also reflect this radiation to an even larger extent. The reflection coefficient of IR radiation by disperse systems greatly depends on their chemical composition. The R values for systems II and III differ by almost an order of magnitude from the R value for system I. Radiation factors also influence the planet's climate through the greenhouse effect. The absorption of polar N_2O molecules by water clusters negligibly changes the effective absorption coefficient of a medium (systems II and III). However, N_2O molecules captured by the clusters do not introduce the same contribution to the greenhouse effect as would be introduced by them in the gaseous state.

Thus, the results of joint study of reflection, absorption, and scattering (reemission) of electromagnetic waves by disperse systems formed by polar molecules indicate the necessity of the account of the effect of the clusterization of greenhouse gases when estimating the greenhouse effect caused by Earth's atmosphere. Among the considered optical processes, the most noticeable influence on the greenhouse effect is caused by the reflection and electric dipole emission and, to a smaller extent, by the absorption of polar molecules by water clusters.

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