
CHEMICAL PHYSICS
OF ATMOSPHERIC PHENOMENA

A Computer Study of Ammonium Adsorption on Water Clusters

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Received June 1, 2012

Abstract—The molecular dynamics method is used to study the adsorption of ammonia on water clusters. The adsorption of ammonia is accompanied by a decrease in the ability of the cluster system to absorb infrared radiation, a significant decline in the thermal radiation power emitted by the system, and an almost double decrease in the frequency-averaged reflection coefficient. An increase in the concentration of ammonia in the clusters causes a slight change in IR absorption coefficient, but enhances the power of emission and reflection coefficient.

Keywords: ammonia, water clusters, the interaction

DOI: 10.1134/S1990793113050047

INTRODUCTION

When dissolved in water, ammonia, a chemical compound of nitrogen and hydrogen (NH_3), yields ammonium hydroxide (NH_4OH_2), which dissociates to the ammonium ion (NH_4^+) and hydroxyl ion (OH^-). Ammonia is of considerable interest, since it plays an important role in the formation of atmospheric aerosols. Aerosols shape the global climate system and influence the weather, changing the temperature and causing precipitations. Aerosols can be of primary origin, i.e., directly emitted in the atmosphere, and of secondary, formed through the conversion of atmospheric gases to solid or liquid particles. The nucleation of secondary aerosols begins with the formation of small clusters of subcritical size. Then, the clusters grow to a critical size and, eventually (typically in the nonequilibrium mode due to changing conditions), become aerosol particles. Experimentally, aerosols larger than 3 nm are mostly studied [1]. Large water clusters, for example, $(\text{H}_2\text{O})_{50}$ (with a transverse size of ~3.5 nm) are present in the clouds [2]. Estimates within the framework of homogeneous nucleation theory suggests that, at the cloud temperature of 233 K the transverse size of the critical nucleus containing ~42 water molecules is 3.3 nm [3]. Water clusters are able to absorb a significant amount of radiant energy, thereby reducing the greenhouse effect (by 3.1 K) [4]. However, so far, they are not included in climate models due to a lack of knowledge about the mechanism of their formation [5]. Based on ab initio calculations, the authors of [6] showed that, ammonium (NH_4^+) hydroxyl (OH^-) ions do not form in clusters containing less than four water molecules. However, already for the $\text{NH}_4^+(\text{H}_2\text{O})_4$ cluster, the transfer of a proton

from a water molecule to the ammonia molecule was observed. Experimental and theoretical studies of the $\text{NH}_4^+(\text{H}_2\text{O})_n$ ($n = 1, 2$) complex revealed the existence of a global energy minimum for the $\text{NH}_4^+(\text{H}_2\text{O})_6$ cluster [7]. The rotational and vibrational frequencies corresponding to this minimum were determined. Monte Carlo simulations in conjunction with density functional theory and steepest descent method made it possible to identify the lowest minima on the potential energy surface of $\text{NH}_4^+(\text{H}_2\text{O})_n$ ($n = 1-4$) clusters [8]. The stabilization of the clusters was provided by hydrogen bonds, and there were a large number of isomers with similar energy. Cyclic structures turned out to be most stable. Clusters containing up to three water molecules had no isomers in which dissociation with the formation of the NH_4^+ and OH^- ions occurred. The dissociation took place in a cluster containing four water molecules, but the energy of the clusters with ions was significantly higher than that of nondissociated clusters. The minimum-energy $\text{NH}_4^+(\text{H}_2\text{O})_4$ cluster had a cyclic structure. The conformational space for ammonia–water clusters is very complex, so it turned out to be impossible, for example, to identify the minimum of the free energy for the $\text{NH}_4^+(\text{H}_2\text{O})_6$ cluster [9]. The behavior of clusters formed in the atmosphere remains unclear. Using molecular dynamics based on quantum-mechanical calculations, the authors of [10] calculated the free energy of the $\text{NH}_4^+(\text{H}_2\text{O})_n$ ($n = 1-10$) clusters, with conflicted with results reported in [8]. According to [10], the free energy of the cluster increases significantly (2.4-fold) in passing from $n = 3$ to $n = 6$. Because clusters with small n are more stable, the authors concluded that a

further growth of ammonia-containing water clusters in the atmosphere should involve other hydrated compounds, such as sulfates, nitrates or chloride anions.

The aim of the present work is to study the absorption capacity of supercritical clusters (containing 50 H₂O molecules) under near atmospheric conditions, calculate the frequency dependence of the absorption and reflection coefficients for infrared radiation and thermal radiation emission spectra.

COMPUTATIONAL MODEL

In this work, we used a new version of the TIP4P model of water [11, 12], taking into account the Lennard-Jones, Coulomb, and polarization interaction. Ammonia–ammonia atom–atom interactions were specified by the Mie–Lennard-Jones and Coulomb contributions:

$$\Phi_{ij}(r) = \varepsilon_{MLJ} \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - 2 \left(\frac{r_0}{r_{ij}} \right)^6 \right] + \frac{q_i q_j}{r_{ij}} \quad (1)$$

The values of ε_{MLJ} , r_0 , and q_i for the H and N atoms of the NH₃ molecule were set equal to 0.038 kcal/mol, 0.28525 nm, 0.333 *e* and 0.41314 kcal/mol, 0.38171 nm, –0.999 *e*, respectively [13]. The Lennard-Jones parameters describing the ammonia–water interaction were calculated by the Berthelot–Lorentz formulas:

$$\varepsilon_{aw}^{(LJ)} = \sqrt{\varepsilon_a^{(LJ)} \varepsilon_w^{(LJ)}}, \quad \sigma_{aw}^{(LJ)} = \frac{\sigma_a^{(LJ)} + \sigma_w^{(LJ)}}{2},$$

where $\varepsilon_a^{(LJ)}$, $\varepsilon_w^{(LJ)}$ and $\sigma_a^{(LJ)}$, $\sigma_w^{(LJ)}$ are the energy and geometric parameters of the potential for the N and H atoms of the ammonia molecule and of the O atom of the water molecule, respectively.

The ammonia molecule has the shape of a trigonal pyramid with the nitrogen atom at the apex. The base of the pyramid is an equilateral triangle formed by the H atoms. The H–N–H bond angle is 107°, which is close to the tetrahedral angle, 109°. The distances between the atoms in the NH₃ molecule are $r_{NH} = 0.102$ nm and $r_{HH} = 0.164$ nm. The NH₃ molecule has a greater polarizability α_p (2.145 Å³) but a smaller dipole moment *d* (1.47 D) as compared to the water molecule (1.49 Å³ and 1.848 D, respectively) [14].

In this work, we used the flexible models of the molecules [15–17], with the deformation of the molecule being determined by balancing the total potential force $\mathbf{f}(\mathbf{u}) = -\frac{\partial \mathbf{r}}{\partial \mathbf{u}} \nabla \Phi(\mathbf{r})$ by the centrifugal force $-\mu \omega^2 \mathbf{u}$, where μ is the reduced mass, *u* is the distance between two atoms, ω is the vibrational frequency, and \mathbf{r} defines the point of application of force.

The integration time step Δt was $0.2 \cdot 10^{-16}$ s. Initially, molecular dynamics calculations for $4 \cdot 10^6 \Delta t$ prepared the equilibrium state at $T = 233$ K for water clusters containing no impurity molecules. The configuration of the (H₂O)_{*n*} cluster at a time of 80 ps was

then used as the starting configuration for simulating the ((NH₃)_{*i*}(H₂O)₅₀) ($1 \leq i \leq 6$) heteroclusters. Each added NH₃ molecule was initially positioned in such a way that the minimum distance between the atoms of this molecule and the atoms of the water molecules be about 0.6 nm. The centers of mass of the NH₃ molecules were placed on the coordinate axes outside the water cluster. The initial orientation of the ammonia molecules was arbitrary. Equilibration the newly formed cluster was performed for at $T = 233$ K, and then, the required physicochemical properties were calculated for $1.2 \cdot 10^6 \Delta t$ at the same temperature. The spectrum of the system was a superposition of the spectra of individual clusters. The next section describes a procedure for determining the number of scattering centers. The average concentration of each type of clusters in the systems under study was by 12 to 13 orders of magnitude smaller than the Loschmidt number.

The equations of motion of the centers of mass of the molecules were integrated using the fourth-order Gear method [18]. The equations of motion for molecular rotation were solved analytically by using the Rodrigues–Hamilton parameters [19], whereas the schema of integration of the equations of motion for rotations was based on the approach proposed by Sonnenschein [20]. The calculations were performed on a PENTIUM-IV computer with a clock frequency of 3.8 GHz.

DIELECTRIC PROPERTIES

Consider the scatter of nonpolarized light at a mean free path *l* of the molecules much smaller than the light wavelength λ . The extinction coefficient (attenuation) ξ of the incident beam can be defined by both the Rayleigh formula [21]

$$\xi = \frac{2\omega^4 (\sqrt{\varepsilon} - 1)^2}{3\pi c^4 N}$$

and the scattering coefficient $\rho \left(\xi = \frac{16\pi}{3} \rho \right)$ [22] in the approximation of scattering at an angle of 90°. Here, *N* is the number of scattering centers in 1 cm³, *c* is the speed of light, ε is the relative permittivity of the medium, and ω is the frequency of the incident wave.

Since $\xi = \alpha + \rho$ (α is absorption coefficient), we have

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

Consider the following types of ultrafine systems:

- (I) a monodisperse system of clusters (H₂O)₅₀;
- (II) a region filled with water clusters containing from 10 to 50 molecules with $\Delta n = 5$;
- (III) a medium consisting of (H₂O)₅₀ clusters adsorbed on one to the six NH₃ molecules.

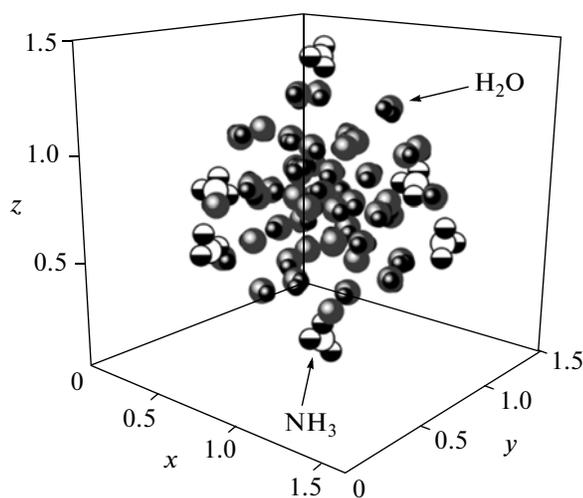


Fig. 1. Configuration of the $(\text{NH}_3)_6(\text{H}_2\text{O})_{50}$ cluster at a time of 100 ps. The coordinates of the molecules are given in nm.

Let us form system III in such a way that the cluster composed of i admixture molecules and n water molecules would have the statistical weight

$$W_{in} = \frac{N_{in}}{N_{\Sigma}}, \quad i = 1 \dots 6, \quad n = 50,$$

where N_{in} is the number of clusters with i admixture molecules and 50 water molecules in 1 cm^3 ; $N_{\Sigma} = \sum_{i=1}^6 N_i$; i can range from 1 to 6. Such weights were used for the $(\text{H}_2\text{O})_n$ clusters comprising system (II). In this case, $i = 0$, whereas n takes values from 10 to 50 at $\Delta n = 5$ steps, so that the upper index in the sum sign is 9. The subsequent calculations of all the spectral characteristics were performed using the specified statistical weights W_{in} .

The static relative permittivity ϵ_0 was calculated from the fluctuations of the total dipole moment [23]. The relative permittivity as a function of frequency $\epsilon(\omega) = \epsilon'(\omega) - i\epsilon''(\omega)$, was calculated by the formula [24, 25]

$$\begin{aligned} \frac{\epsilon(\omega) - 1}{\epsilon_0 - 1} &= - \int_0^{\infty} \exp(-i\omega t) \frac{dF}{dt} dt \\ &= 1 - i\omega \int_0^{\infty} \exp(-i\omega t) F(t) dt, \end{aligned}$$

where the function $F(t)$ is the normalized autocorrelation function of the total dipole moment of the cluster:

$$F(t) = \frac{\langle \mathbf{d}_{cl}(t) \mathbf{d}_{cl}(0) \rangle}{\langle \mathbf{d}_{cl}^2 \rangle}.$$

The absorption coefficient α of external IR radiation can be expressed through the imaginary part of the frequency-dependent relative permittivity $\epsilon(\omega)$ as [26]

$$\alpha(\omega) = 2 \frac{\omega}{c} \text{Im} [\epsilon(\omega)^{1/2}].$$

The reflection coefficient R was defined as the ratio of the average reflected energy flux to the incident flux. For normal incidence of a monochromatic plane wave, the reflection coefficient is given by [21]

$$R = \frac{|\sqrt{\epsilon_1} - \sqrt{\epsilon_2}|^2}{|\sqrt{\epsilon_1} + \sqrt{\epsilon_2}|^2}. \quad (2)$$

In deriving this formula, it was assumed that the wave propagates from a transparent medium (medium 1) into a medium that can be both transparent and non-transparent, i.e., absorbing and scattering (medium 2). The subscripts on the relative permittivity in (2) indicate the medium.

The frequency dispersion of the relative permittivity determines the frequency dependence of the dielectric loss $P(\omega)$ as [22]

$$P = \frac{\epsilon'' \langle E^2 \rangle \omega}{4\pi},$$

where $\langle E^2 \rangle$ is the average of the square of the electric field strength and ω is the frequency of the emitted electromagnetic wave.

CALCULATION RESULTS

The configuration of the $(\text{NH}_3)_6(\text{H}_2\text{O})_{50}$ cluster obtained at a time of 50 ps is shown in Fig. 1. As can be seen, by this time, all six NH_3 molecules closely approached the surface of the $(\text{H}_2\text{O})_{50}$ cluster and occupied definite positions, being bound to one or two water molecules. The orientation of the NH_3 molecule relative to the fixed xyz coordinate system is rather arbitrary. However, it is seen that the N atom tends to approach one of the H atoms of the nearest water molecule, whereas the O atom of the neighboring water molecule tends to get closer to one of the H atoms of the NH_3 molecule. This demonstrates how new hydrogen bonds are formed in the cluster, being accompanied, of course, by the cleavage of some former hydrogen bonds between H_2O molecules.

The real and imaginary parts of the relative permittivity of a system composed of water clusters depend on their size. Curves 1 and 2 in Fig. 2 characterize the frequency dependence of the complex relative permittivity of systems consisting of $(\text{H}_2\text{O})_n$ clusters: (1) $n = 50$ (system I) and (2) $n = 10-50$ (system II). At frequencies of $\omega < 3200 \text{ cm}^{-1}$, the values of ϵ' and ϵ'' for system I, consisting generally of larger clusters, is higher than for system II. The adsorption of NH_3 molecules by water clusters, i.e., transition to system III, leads to a significant decrease in the values of ϵ' and ϵ'' (curve 3). On average, in the frequency range of 0 to 3500 cm^{-1} ,

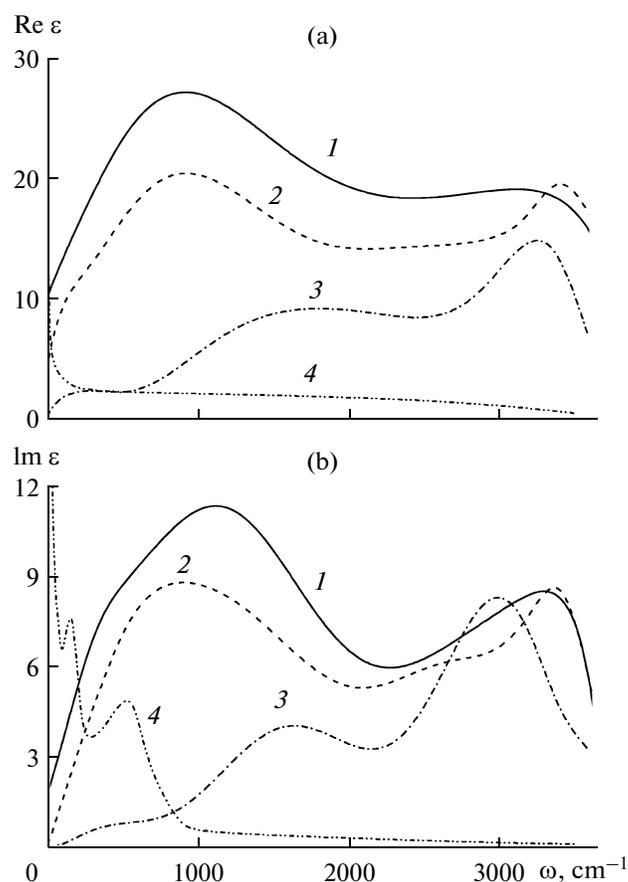


Fig. 2. (a) Real (MD calculation [26]) and (b) imaginary (experiment [27]) parts of the relative permittivity of various systems of clusters: (1) $(\text{H}_2\text{O})_n = 50$ (system I), (2) $(\text{H}_2\text{O})_n = 10, \dots, 50$ (II), (3) $(\text{NH}_3)_i = 1, \dots, 6(\text{H}_2\text{O})_{50}$ (III), and (4) bulk water.

the values of ϵ' for system III decreased 2.7-fold as compared to system I and 2.1-fold relative to system II; the values of ϵ'' decreased respectively by factors of 2.2 and 1.8. The values of ϵ' and ϵ'' for the system of clusters containing NH_3 molecules (system III) are higher than the corresponding quantities for bulk water [26, 27] at $\omega > 550$ and $\omega > 820 \text{ cm}^{-1}$, respectively. The significant decrease in the values of ϵ' and ϵ'' for the ensemble of clusters that adsorbed NH_3 molecules is associated with a loosening of the structure due to a rearrangement of the hydrogen bonds.

The individual IR absorption coefficient spectra of the $((\text{NH}_3)_i(\text{H}_2\text{O})_{50})$ ($i = 1, \dots, 6$) are shown in Fig. 3. As can be seen, the addition of NH_3 molecules to the water cluster only slightly alters both the form and intensity of the $\alpha(\omega)$ spectrum. The main peak of the spectrum is located at 3349 cm^{-1} at all i except for $i = 4$, where the spectrum peak is shifted to lower frequencies (3307 cm^{-1}), whereas the integrated intensity of the IR spectrum changes only within 6% as the number of adsorbed NH_3 molecules is varied from 1 to 6. The adsorption of any number of NH_3 molecules within $i = 1-6 \text{ NH}_3$ leads to a decrease in the intensity of infrared radiation absorption. Consequently, the

spectrum of the monodisperse ensemble of pure water clusters (system I) has a markedly higher intensity (1.45-fold) than the corresponding spectrum of sys-

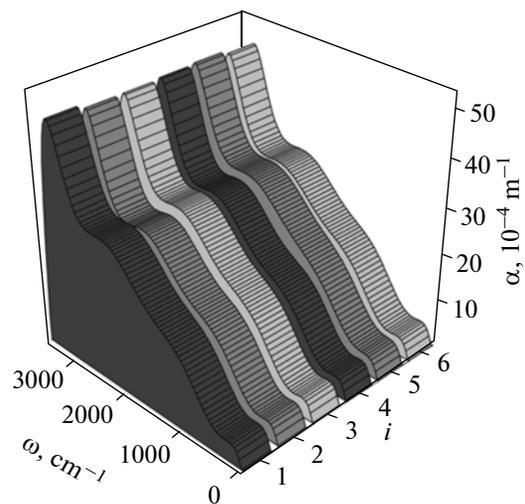


Fig. 3. IR absorption spectra of the $(\text{NH}_3)_i(\text{H}_2\text{O})_{50}$ ($1 \leq i \leq 6$) clusters.

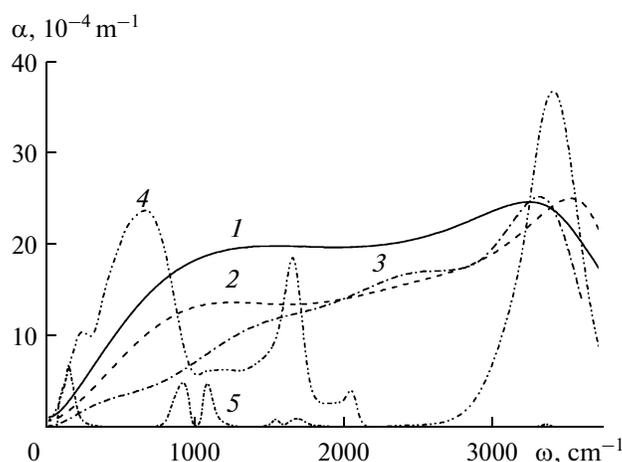


Fig. 4. IR absorption spectra for various systems: (1) $(\text{H}_2\text{O})_{50}$ cluster, (2) $(\text{H}_2\text{O})_n$ ($10 \leq n \leq 50$), (3) $(\text{NH}_3)_i(\text{H}_2\text{O})_{50}$ ($1 \leq i \leq 6$), (4) $\alpha(\omega)$ function for bulk water (experiment [28]), and (5) gaseous NH_3 (experiment [29]).

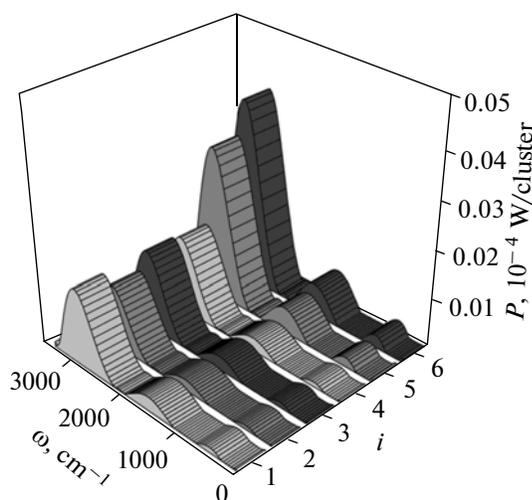


Fig. 5. IR emission spectra of the $(\text{NH}_3)_i(\text{H}_2\text{O})_{50}$ ($1 \leq i \leq 6$) clusters.

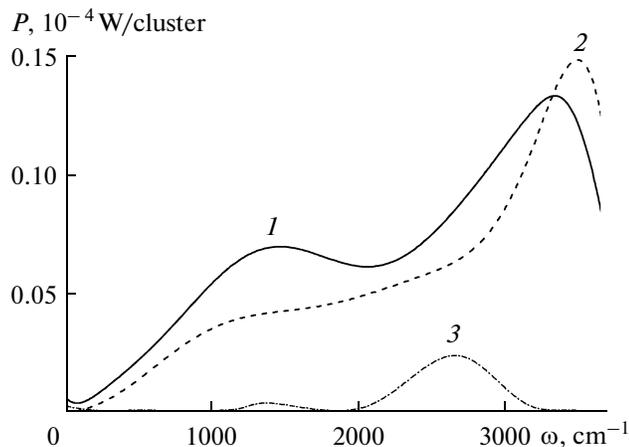


Fig. 6. IR emission spectra for various systems: (1) $(\text{H}_2\text{O})_{50}$ cluster, (2) $(\text{H}_2\text{O})_n$ ($10 \leq n \leq 50$), and (3) $(\text{NH}_3)_i(\text{H}_2\text{O})_{50}$ ($1 \leq i \leq 6$).

tem III, consisting of clusters of water molecules with captured NH_3 molecules (Fig. 4). Moreover, the system of water clusters composed of different much smaller clusters (system II) has the integrated intensity of infrared radiation absorption by a factor of 1.1 higher than that of system III. The main peak of the spectrum of system III has a red shift of 89 cm^{-1} relative to the corresponding experimental spectrum of liquid water [28]. The position of the second peak (1650 cm^{-1}) of this spectrum of liquid water is close to the point of inflection in the $\alpha(\omega)$ curve for system III. All the major peaks in the infrared spectrum of gaseous NH_3 are located in the frequency range of $\omega < 1700 \text{ cm}^{-1}$ [29]. The positions of the second and third peaks of the $\alpha(\omega)$ spectrum of gaseous ammonia occurs in the region of considerable growth of the intensity of the respective spectrum for system III. Thus, the adsorption of NH_3 molecule by water clusters leads to a weakening of the ability of disperse aquatic media to absorb infrared radiation.

The shape of the individual emission spectra of water clusters with adsorbed ammonia molecules is much of the same type (Fig. 5). The integrated intensity of the emission spectra of the $((\text{NH}_3)_i(\text{H}_2\text{O})_{50})$ ($i = 1-6$) clusters changes more significantly upon addition of NH_3 molecules than the absorption spectra do. For example, the cluster with six ammonia molecules emits 3 times more radiation than the cluster with two adsorbed NH_3 molecules. In all the cases, the emission is most intense at a frequency of 2887 cm^{-1} ; i.e., the main emission frequency is lower than the main absorption frequency. Thus, the model features a random emission of infrared radiation by clusters [30].

The integrated intensity of the emission spectrum of monodisperse pure water clusters of (system I) is 1.2 times higher than the respective characteristic of smaller water clusters (system II). At the same time, the integrated intensities of the $P(\omega)$ spectra for sys-

tems I and II are far superior (by factors of 12.6 and 10.6, respectively) to system III in I_p value. The main peak of the $P(\omega)$ spectrum of system II exhibits a blue shift of 150 cm^{-1} relative to the respective peak of the corresponding spectrum of system I. The most intense peak of the $P(\omega)$ spectrum of III system features a red shift (by 675 and 825 cm^{-1}) relative to the respective peaks in the $P(\omega)$ spectra of systems I and II. The second major peak in the emission spectrum of system III is shifted to lower frequencies by $\sim 70\text{ cm}^{-1}$ with respect to the corresponding peak of system I. System II has a unimodal $P(\omega)$ spectrum.

The individual IR reflection spectra of the $((\text{NH}_3)_i(\text{H}_2\text{O})_{50}, i = 1, \dots, 6)$ have a jagged shape, differing from each other in intensity (Fig. 7). The reflection spectrum intensity of the cluster with six NH_3 molecules exceeds that for the cluster with two ammonia molecules by a factor of almost 2. The main peak of the $R(\omega)$ spectrum does not change its position upon addition of ammonia molecules to the cluster, remaining at 2835 cm^{-1} .

The reflection spectrum of system II (Fig. 8a) is suggestive of a sufficiently smooth frequency dependence of the reflection coefficient, as is the case with system I, the $R(\omega)$ spectrum of which is approximated by curve 2 in Fig. 8b. The reflection spectrum $R(\omega)$ changes significantly upon adsorption of molecules NH_3 on the water clusters (Fig. 8b, histogram 1). The $R(\omega)$ spectrum of system III is highly jagged. Most of the spectrum has a low intensity. Against this background, there are several high-intensity peaks. In general, the integrated intensity of the $R(\omega)$ spectrum of system III is almost two times lower than that of the corresponding spectrum of system I, and 1.7 times lower than that of the $R(\omega)$ spectrum of system II. In addition, the adsorption of ammonia molecules changes the nature of infrared radiation reflection. While for the system of pure water clusters, the reflection maximum is located near 1000 cm^{-1} , for system III, it is shifted to 2835 cm^{-1} . The observed changes in the $R(\omega)$ spectrum of system III indicate a strong change in the structure of the surface of the water clusters after adsorption on them of NH_3 molecules, which make ammonia adsorption very different from ozone adsorption [31].

CONCLUSIONS

In the present work, the possibility of the donor–acceptor interaction of ammonia with the surface of water clusters was demonstrated. The molecular dynamics method was used to study the spectral characteristics of a system of water clusters with adsorbed ammonia molecules. The maximum concentration of ammonia in the clusters was significantly (more than fourfold) lower than the maximum concentration of ammonia in aqueous solution. In areas with the largest natural concentration of ammonia in the atmosphere,

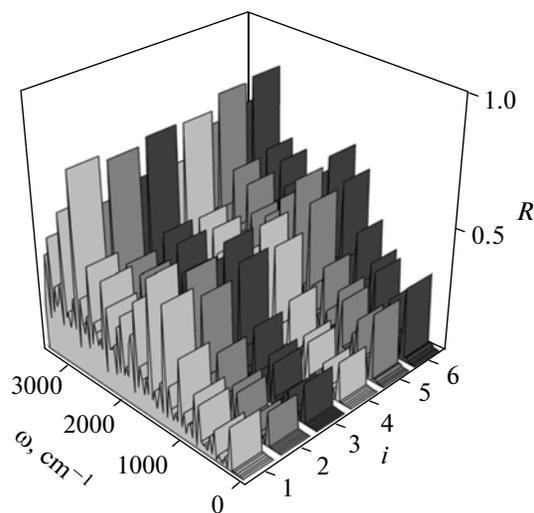


Fig. 7. Reflection coefficients of a monochromatic electromagnetic wave normally incident on the surface of the $(\text{NH}_3)_i(\text{H}_2\text{O})_{50}$ ($1 \leq i \leq 6$) clusters.

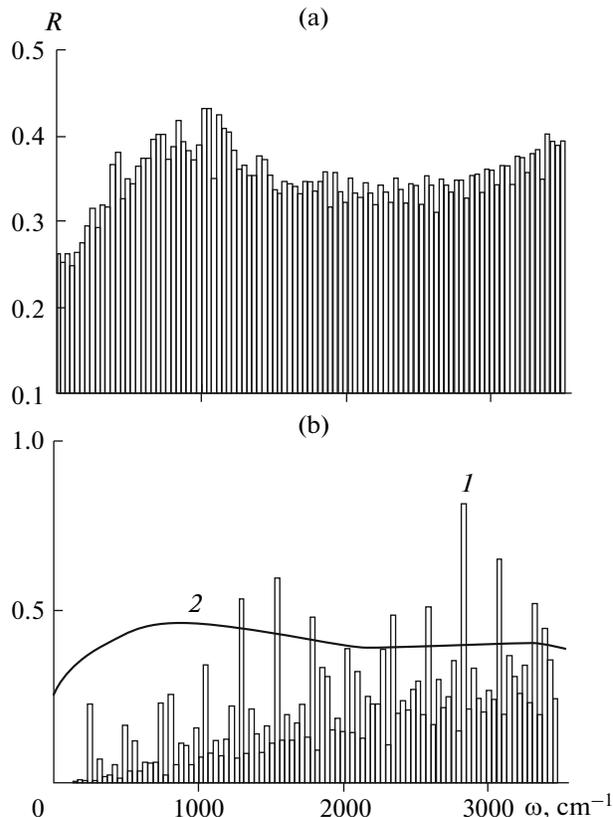


Fig. 8. Reflection coefficients of (a) $(\text{H}_2\text{O})_n$ ($10 \leq n \leq 50$) and (b) (1) $(\text{NH}_3)_i(\text{H}_2\text{O})_{50}$ ($1 \leq i \leq 6$) and (2) $(\text{H}_2\text{O})_{50}$ clusters.

for each NH_3 molecule, there are up to H_2O molecules. Therefore, the formation of water clusters and adsorption of ammonium molecules on them is quite likely. The real and imaginary parts of the permittivity determine respectively the refractive index and the

absorption coefficient (optical constants) of the medium. These quantities are not independent of one another. The reduction in the values of ε' and ε'' due to the adsorption of ammonia by the dispersed aqueous medium results in a decrease of the refractive indices and absorption coefficient; i.e., the medium becomes optically less dense, so the rate of attenuation of an electromagnetic wave decreases. Addition of ammonia molecules to the clusters weakens their ability to absorb infrared radiation. Note that the absorbance of the clusters does not depend significantly on the number of adsorbed ammonia molecules. The adsorption of ammonia causes a substantial decrease in the power of infrared radiation emitted by the clusters. However, at a large concentration of ammonia in the water clusters, the emission power increases. The system of water clusters with adsorbed ammonium molecules significantly reduces the ability to reflect infrared radiation. The maximum of reflection shifts to higher frequencies with respect to the main peak in the corresponding spectrum of pure water clusters. However, high concentrations of ammonia in the clusters enhance their reflectivity.

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Translated by V. Smirnov