Computer study of the formation of water–ammonia clusters and their dielectric properties

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The absorption of one to six ammonia molecules by the $(H_2O)_{50}$ cluster is studied by the molecular dynamics method under near-atmospheric conditions. The capture of NH_3 molecules by a water cluster produces an increase in the integrated intensity of IR absorbance, substantially decreases emission power in the frequency range of $0 \leq \omega \leq 3500$ cm^{-1}, and transforms a continuous reflectance spectrum into a banded one. Adsorption of ammonia molecules by water clusters greatly diminishes the number of electrons that are active with respect to electromagnetic radiation. The present results are also compared with the experimental findings wherever available.

Keywords: ammonia, water cluster, infrared absorption spectra, molecular dynamics

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1. Introduction

Ammonia is the most significant alkaline compound found in the atmosphere, which readily neutralizes strong inorganic acids such as sulfuric, hydrochloric, and nitric acids. Ammonia has a noticeable effect on atmospheric processes because of its high valence, which determines its role as a potential site of proton sink and ionic nucleation. The combined action of ammonia and sulfuric acid enhances atmospheric nucleation. Ammonia plays an important role in the chemistry of the cloud layers of Jupiter and Saturn, and a substantial amount of ammonia has been found on Uranus and Neptune.[1] The interaction of ammonia with water yields ammonium hydroxides. Under normal conditions, saturated ammonia solutions are characterized by an NH_3 to H_2O ratio of 1 mol:1 mol. Strong cooling of such a solution (to about 190 K) gives rise to the crystallization of ammonia hydrate $NH_3 \cdot H_2O$. Hydrate of the $NH_3 \cdot 2H_2O$ composition (dihydrate) is known to prevail at low pressures.

The interest in the spectroscopic properties of molecular aggregates arises from their growing relevance in many different fields. They range from medical applications,[2] to atmospheric processes[3] and astrophysics.[4] Intrinsic particle properties such as the particle size, the particle shape, or structural changes in the particle's surface characteristically influence the vibrational dynamics of these aggregates. So far, it is still a challenge to understand such intrinsic particle properties on a microscopic level, that means in terms of inter- and intramolecular interactions. In the nanometer size range (about 1 nm–10 nm), the influence of the particle surface is no longer negligible. For the smallest particles, the portion of surface molecules can even dominate over the portion of molecules in the interior of the particle. Because the particle surface in general has not the same structure as the interior this can lead to characteristic surface absorption. Such phenomena have been investigated by Devlin and Buch for the example of small ice particles by combining infrared spectroscopy with extensive calculations.[5]

At present, mathematical simulation is the main source of information on the infrared band intensities of the clusters.[6] Direct measurement of this characteristic is, in most cases, complicated by the difficulties connected to the determination of the absolute number density. The strong enhancement of the infrared band intensities of different hydrogen-bonded clusters suspended in a cryogenic matrix was discovered several-dozen years ago.[7] However, the spectrum broadening and the complex kinetic of cluster formation in solid matrices made it impossible to determine this characteristic for clusters of a certain size. This problem was solved using the technique of encapsulation into helium droplets.[8] The quantum nature of helium droplets at very low temperatures enabled researchers to form molecular clusters and avoid spectral broadening.

The goal of this work is to study the optical effects resulting from adsorption of ammonia molecules by large water clusters (these effects manifesting themselves as changes in the spectra of IR absorption, emission, and reflection).

2. Molecular dynamics model

The interaction of water molecules in clusters is described by a nonadditive potential, the additive component of which is represented by the modified[9] TIP4P potential for water,[10] while its nonadditive component is determined by the polarization interaction.[11]

The ammonia–ammonia interatomic interactions are determined by the Lennard–Jones and Coulomb contributions as

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follows:

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

The magnitudes of parameters ε_{ij}, r_0, and q_i of H and N atoms in the NH_3 molecule equal to 0.159 kJ/mol, 0.28525 nm, 0.333e and 1.730 kJ/mol, 0.38171 nm, 0.999e, respectively.[12] The parameters of the Lennard–Jones potential that describes the ammonia–water interaction were found by the Berthelot–Lorentz formulas

$$\varepsilon_{\mathrm{aw}}^{(\mathrm{LJ})} = \sqrt{\varepsilon_{\mathrm{a}}^{(\mathrm{LJ})}\varepsilon_{\mathrm{w}}^{(\mathrm{LJ})}}, \quad \sigma_{\mathrm{aw}}^{(\mathrm{LJ})} = \frac{\sigma_{\mathrm{a}}^{(\mathrm{LJ})} + \sigma_{\mathrm{w}}^{(\mathrm{LJ})}}{2}, \quad (2)$$

where $\varepsilon_{\mathrm{a}}^{(\mathrm{LJ})}$ and $\varepsilon_{\mathrm{w}}^{(\mathrm{LJ})}$ are the energy parameters and $\sigma_{\mathrm{a}}^{(\mathrm{LJ})}$ and $\sigma_{\mathrm{w}}^{(\mathrm{LJ})}$ are the geometric parameters of the potential for N and H atoms of the ammonia molecule and O atom of the water molecule, respectively.

The ammonia molecule has the shape of a triangular pyramid, with a nitrogen atom occurring at the vertex. The base of the pyramid represents an equilateral triangle formed by H atoms. The H–N–H bond angle is 107°, which is close to the tetrahedral angle of 109°. The interatomic distances in the NH_3 molecule are $r_{\mathrm{NH}} = 0.102$ nm and $r_{\mathrm{HH}} = 0.164$ nm. The NH_3 molecule has a higher polarizability α^{p} (2.145 Å^3, 1 Å = 0.1 nm) and lower dipole moment d (1.47 D, 1 D$=$ 3.33564×10^{-30}C·m) than does the water molecule (1.49 Å^3 and 1.848 D), respectively.[13]

The trajectories of the centers of masses of molecules were determined by the fourth-order Gear method in Ref. [14]. Time step Δt of integration is 0.2×10^{-16} s. In a molecular-kinetic calculation $4\times10^6\Delta t$ long, the equilibration is preliminarily performed at $T = 233$ K for pure water clusters free of impurity molecules. The $(H_2O)_n$ cluster configuration corresponding to the time moment of 80 ps is further used as the initial configuration for simulating $(NH_3)_i(H_2O)_{50}$ heteroclusters with $1 \le i \le 6$. Each added NH_3 molecule was initially placed into a position such that the shortest distance between the atoms of this molecule and atoms of water molecules was about 0.6 nm. At the beginning, the centers of masses of NH_3 molecules were placed in the coordinate axes outside the water cluster. The initial orientation of ammonia molecules was arbitrary. A newly formed cluster was equilibrated within a time interval of $1.2\times10^6\Delta t$ at $T = 233$ K; then, the desired physicochemical properties were calculated at the same temperature for $2.5\times10^6\Delta t$.

A system of $(NH_3)_i(H_2O)_{50}$ clusters was formed in accordance with cluster statistical weights, which were determined as follows. Let us consider the case of unpolarized light scattering when the free path l of molecules is much shorter than the light wavelength λ. The extinction (attenuation) ratio h of an incident beam is determined by, on the one hand, the Rayleigh formula[15] and, on the other hand, scattering coefficient ρ ($h = 16\pi\rho/3$)[16] under an approximation of the scattering angle of 90°. Taking into account that $h = \alpha + \rho$, where α is the absorption coefficient, we have

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

where N is the number of scattering centers per cubic centimeter, c is the speed of light, ε is the medium dielectric permittivity, and ω is the incident wave frequency. We will assume that system I is a monodisperse system of clusters $(H_2O)_{50}$. Let us form systems II and III from $(H_2O)_n$ and $(NH_3)_i(H_2O)_{50}$ clusters, respectively, in a manner such that a cluster containing i impurity molecules and n water molecules has the following statistical weight:

$$W_{\mathrm{in}} = \frac{N_{\mathrm{in}}}{N_\Sigma}, \quad 1 \le i \le 6, \quad 10 \le n \le 50 \ \ (\Delta n = 5), \quad (4)$$

where N_{in} is the number of clusters containing a number n of water molecules and a number i of NH_3 molecules per cubic centimeter, $N_{1\Sigma} = \sum_{n=1}^{9} N_{i=0,n}$, $N_{2\Sigma} = \sum_{i=1}^{6} N_{i,n=50}$. Then, all spectral characteristics were calculated with allowance for the accepted statistical weights W_{in}. The equations of motion for molecule rotation were analytically solved using the Rodrigues–Hamilton parameters,[17] while the equations of motion involving rotations were integrated according to the Sonnenschein approach.[18]

3. Dielectric properties

The total dipole moment $\boldsymbol{d}_{\mathrm{cl}}$ of a cluster is calculated by the following formula:

$$\boldsymbol{d}_{\mathrm{cl}}(t) = Z_+\sum_{i=1}^{N_{\mathrm{tot1}}}\boldsymbol{r}_i(t) + Z_-\sum_{j=1}^{N_{\mathrm{tot2}}}\boldsymbol{r}_j(t), \quad (5)$$

where $\boldsymbol{r}_i(t)$ is the vector indicating the location of atom i or point M at time t; Z is the electric charge located in the center under consideration; subscript "+" refers to H atoms, which carry positive electric charges; subscript "–" refers to points M or N atoms; and N_{tot1} and N_{tot2} are the numbers of positively and negatively charged atoms in the cluster, respectively. Static dielectric constant ε_0 is calculated via the fluctuations of total dipole moment[19] as follows:

$$\varepsilon_0 = 1 + \frac{4\pi}{3VkT}\left[\langle \boldsymbol{d}_{\mathrm{cl}}^2\rangle - \langle \boldsymbol{d}_{\mathrm{cl}}\rangle^2\right], \quad (6)$$

where V is the cluster volume and k is Boltzmann's constant.

Dielectric permittivity $\varepsilon(\omega)$ as a function of frequency ω is expressed by complex value $\varepsilon(\omega) = \varepsilon'(\omega) - \mathrm{i}\varepsilon''(\omega)$ which is determined using the following equation:[19,20]

$$\frac{\varepsilon(\omega)-1}{\varepsilon_0-1} = -\int_0^\infty \exp(-\mathrm{i}\omega t)\frac{\mathrm{d}F}{\mathrm{d}t}\mathrm{d}t$$

$$= 1 - \mathrm{i}\omega \int_0^\infty \exp(-\mathrm{i}\omega t) F(t)\,\mathrm{d}t, \tag{7}$$

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

$$F(t) = \frac{\langle \boldsymbol{d}_{\mathrm{cl}}(t) \cdot \boldsymbol{d}_{\mathrm{cl}}(0) \rangle}{\langle \boldsymbol{d}_{\mathrm{cl}}^2 \rangle}. \tag{8}$$

If the dipole moments of molecules have been determined, the IR absorption cross section is defined as follows:[21]

$$\sigma(\omega) = \left(\frac{2}{\varepsilon_v c \hbar n}\right) \omega \tanh\left(\frac{\hbar\omega}{2kT}\right) \times \mathrm{Re} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \langle \boldsymbol{d}_{\mathrm{cl}}(t) \cdot \boldsymbol{d}_{\mathrm{cl}}(0) \rangle, \tag{9}$$

where n is the frequency-independent refractive index, ε_v is the dielectric permittivity of a vacuum, and c is the speed of light.

Reflection coefficient R is defined as the ratio between the average energy flux reflected from a surface and the incident flux. At the normal incidence of a plane monochromatic wave, the reflection coefficient is determined by the following formula:[15]

$$R = \left| \frac{\sqrt{|\varepsilon_1|} - \sqrt{|\varepsilon_2|}}{\sqrt{|\varepsilon_1|} + \sqrt{|\varepsilon_2|}} \right|^2. \tag{10}$$

Here, it is assumed that the wave incidence occurs from a transparent medium (medium 1) into a medium that may be both transparent and nontransparent, i.e., an absorbing and scattering medium (medium 2). The subscripts at the dielectric permittivity in expression (10) denote the media.

The frequency dispersion of the dielectric permittivity determines the frequency dependence of dielectric loss $P(\omega)$ according to the following expression:[16]

$$P = \frac{\varepsilon'' \langle E^2 \rangle \omega}{4\pi}, \tag{11}$$

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

Total number N_{el} of electrons in cluster unit volume that interact with an external electromagnetic field is defined in the following form:[15]

$$N_{\mathrm{el}} = \frac{m}{2\pi^2 e^2} \int_0^\infty \omega \varepsilon''(\omega)\,\mathrm{d}\omega, \tag{12}$$

where e and m are the electron charge and mass, respectively.

Motion at a frequency lower than 1200 cm^{-1} corresponds to librations of molecules, while frequencies higher than 1200 cm^{-1} mainly describe intramolecular vibrations,[22] which are realized in the following approximation.

Flexible models of molecules are considered. Molecules are provided with flexibility via the procedure that had been developed within the framework of the Hamilton dynamics.[23,24] Let us consider a diatomic molecule. Assume that atoms a and b in a molecule are separated by a distance of

$$Q = \|\boldsymbol{r}_a - \boldsymbol{r}_b\|, \tag{13}$$

where $\boldsymbol{r}_a$ and $\boldsymbol{r}_b$ are the position vectors of the atoms. We denote the corresponding velocities as $\boldsymbol{v}_a$ and $\boldsymbol{v}_b$ and express the reduced mass as

$$\mu = \frac{m_a m_b}{m_a + m_b}. \tag{14}$$

The size of the molecule represented by atoms a and b is determined by balancing total potential force $\boldsymbol{f}(\boldsymbol{Q}) = -(\partial \boldsymbol{r}/\partial \boldsymbol{Q})\nabla\Phi(\boldsymbol{r})$ with centrifugal force $-\mu Q\omega^2$, so that

$$-\mu Q\omega^2 - \boldsymbol{f}(\boldsymbol{r}) \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{Q}} = 0, \tag{15}$$

where $\omega = \|\boldsymbol{v}_a - \boldsymbol{v}_b\|/Q$ is the angular velocity. Minimizing the contribution of each generalized coordinate to potential energy U, we obtain

$$\frac{\partial}{\partial Q_i} H(\boldsymbol{r}, \boldsymbol{v}) = \frac{\partial}{\partial Q_i} \left(\frac{1}{2} \mu_i Q_i^2 \omega_i^2 + U(\boldsymbol{r}) \right) = 0. \tag{16}$$

This method can be generalized for molecules of any composition.[25]

4. Results

The configuration of a $5\mathrm{NH_3} + (\mathrm{H_2O})_{50}$ system at the 50 ps time moment is illustrated in Fig. 1. It can be seen that, by this time moment, all five ammonia molecules have been absorbed by the water cluster. NH_3 molecules have different orientations; however, as a rule, they tend to be arranged in a manner such that an N atom is hydrogen-bonded with a water molecule. In turn, H atoms of NH_3 molecules "seek" oxygen atoms of water molecules. In a formed $(NH_3)_5(H_2O)_{50}$ cluster, NH_3 molecules remain on the aggregate surface. A newly formed $\mathrm{N}\cdots\mathrm{H}$ hydrogen bond cannot rupture the network of hydrogen bonds of a dense water core in the cluster center, and the NH_3 molecule cannot penetrate into the aggregate.

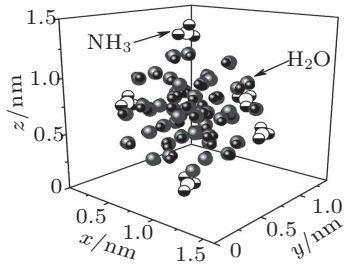


Fig. 1. Configuration of $(NH_3)_5(H_2O)_{50}$ cluster at the 50-ps time moment.

The IR adsorption spectra calculated for systems I–III, together with the corresponding experimental spectra of liquid water[26] and gaseous ammonia,[27] are shown in Fig. 2. Note that, in the frequency range of $0 \leq \omega \leq 3600$ cm^{-1}, the spectrum of system II is more intense (by a factor of 1.4) than the corresponding spectrum of system I. It is of interest that the IR spectrum intensity for system III is 2.7 times higher than that for system II. This is related to not only the larger sizes of clusters in system III, but also the inhibition of vibrations due to the formation of additional N$\cdots$H hydrogen bonds. The main peak in the spectrum of system III exhibits a red shift by 610 cm^{-1} relative to the corresponding peak of system II. In turn, the main peak in the IR spectrum of system II is characterized by a blue shift by 70 cm^{-1} with respect to the main peak of bulk liquid water. The second peak in the IR spectrum of system III is located at 1546 cm^{-1}, i.e., close to one of the doubled peaks in the IR spectrum of gaseous NH_3 (1530 cm^{-1}). Another peak of this doublet corresponds to a frequency of 1680 cm^{-1}. In the IR spectrum of system II, the second and other peaks cannot be revealed in the scale of Fig. 2. The added NH_3 molecules enhance the orientational order in the clusters to markedly increase the correlation time of the cluster dipole moments and, as a result, the intensities of the IR absorption spectra.

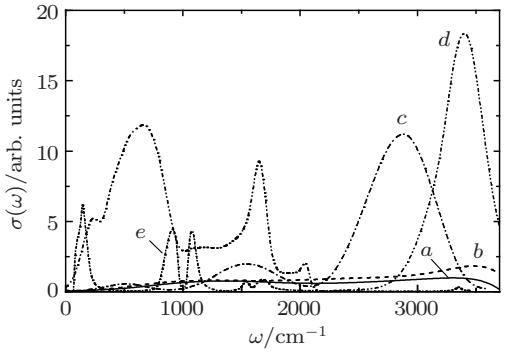


Fig. 2. IR absorption spectra of cluster systems: system I (curve *a*), system II (curve *b*), sytem III (curve *c*), experimental data on for bulk liquid water (curve *d*),[26] and experimental spectrum of gaseous NH_3 (curve *e*). [27]

The integral power $P(\omega)$ of IR radiation emitted by a monodisperse system of water clusters (system I) is 1.3 times higher than that of the system composed of water clusters of nine different sizes (system II) as shown in Fig. 3. System I is characterized by a bimodal spectrum, the main maximum of which corresponds to frequency $\omega = 3340$ cm^{-1}, while system II exhibits a unimodal spectrum with the main maximum at $\omega = 3495$ cm^{-1}. A great decrease (by a factor of 10.6) is observed in the intensity of the $P(\omega)$ emission spectrum of system III relative to that of system II. The location of the maximum in the $P(\omega)$ spectrum of system III shifts toward lower frequencies by 830 cm^{-1} relative to the corresponding spectrum of system II. The main emission frequency of system III (ω_P =2667 cm^{-1}) is lower than the main frequency of absorption (ω_σ =2879 cm^{-1}) by 212 cm^{-1}. This indicates a spontaneous character of IR radiation emission by $(NH_3)_i(H_2O)_{50}$ clusters. An analogous conclusion can be drawn from a comparison of the $\sigma(\omega)$ and $P(\omega)$ spectra for system II, but, in this case, the difference in the main frequencies is not so large (10 cm^{-1}). The weakening of hydrogen bonds in clusters as a result of adsorption of NH_3 molecules drastically reduces the intensity of the cluster emission spectra and, hence, their visibility.

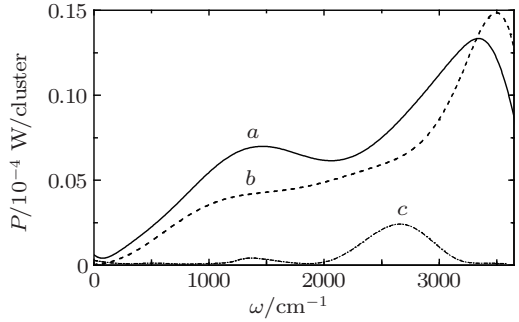


Fig. 3. IR emission spectra for different systems: system I (curve *a*), system II (curve *b*), and system III (curve *c*).

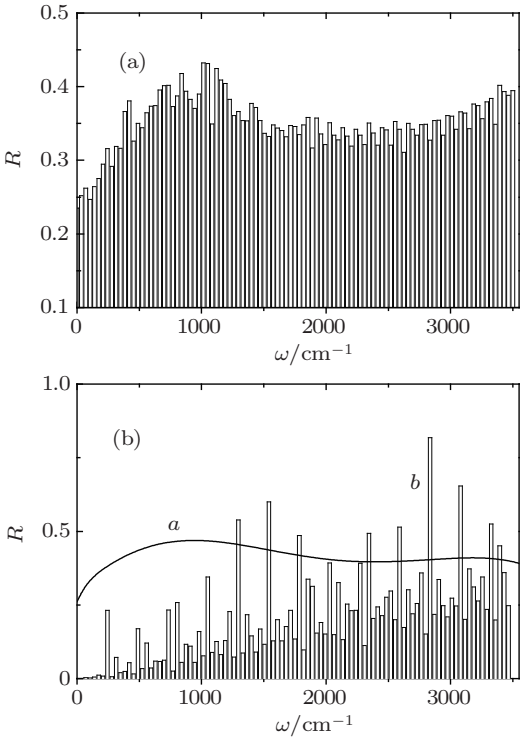


Fig. 4. Coefficients of monochromatic plane electromagnetic wave reflection by different disperse systems: (a) system II, (b) system I (curve *a*) and system III (curve *b*).

The IR reflection spectra $R(\omega)$ of systems I and II are continuous, while that of system III is almost banded as shown in Fig. 4. The average values of reflection coefficient $\bar{R}$ for systems of pure water clusters (systems I and II) are 0.40 and 0.35, respectively, while that of water clusters containing adsorbed ammonia molecules (system III) is 0.20. The substantial reduction in the reflection ability of a system of water clusters

after adsorption of NH_3 molecules by the clusters is caused by the formation of a strongly rough surface. Reflected IR radiation maxima of systems I and II correspond to 945 cm^{-1} and 1012 cm^{-1}, respectively, while that of system III is observed at 2835 cm^{-1}.

For ammonia, not only the boiling and melting temperatures, but also the conductivity and dielectric permittivity, are lower than those for water. Ammonia is easily transformed into a colorless liquid, which strongly refracts light. Hydrogen bonds in liquid ammonia with a density of 0.6814 g/cm^3 are much weaker than in water. Ammonia molecule contains only one lone–electron pair in contrast to two pairs in water molecule. This circumstance makes the formation of a branched network of hydrogen bonds between several molecules impossible. Due to the hydrogen bonding, liquid ammonia is, similarly to water, strongly associated and actually nonconducting. Impurities that increase and decrease the number N_{el} of free electrons are referred to as donors and acceptors, respectively. Upon ionization of an acceptor impurity, electrons are captured from the valence region. Acceptor impurities with ionization energy on the order of thermal energy kT are described by a hydrogen-like model.

The oxidation state of nitrogen atoms is minimum (-3) in ammonia. While, in nitrate radicals, it is maximum (+5). Nitrogen has eight intermediate oxidation states between these extrema. It is of interest to compare (Fig. 5) the dependences of the number N_{el} of electrons involved in the interaction with electromagnetic radiation on the number i of NH_3 molecules (curve a in Fig. 5) and nitrate ions (curve b in Fig. 5) captured by a water cluster. As a whole, the behaviors of the $N_{el}(i)$ dependences upon the adsorption of these two nitrogen-containing components are identical, with the exception of slight differences observed in the range of $1 \leq i \leq 4$. In both cases, the primary addition of ammonia molecules and NO_3^- ions to a water aggregate causes a strong (by tens of times) reduction in the N_{el} value. The small numbers of electrons that interact with light remain preserved up to the addition of four NH_3 molecules to a water cluster. When the fifth and sixth ammonia molecules are added to the cluster, a tendency toward an increase in N_{el} is observed. However, this increase is insubstantial as compared with the reduction in N_{el} caused by the primary addition of NH_3 molecules to water clusters. As a rule, adsorption of nitrate ions induces larger fluctuations in the number of electromagnetically active electrons than does the adsorption of NH_3 molecules. Upon the adsorption of two, three, five, and six ions, N_{el} increases, while, upon the addition of four ions, it decreases. However, in no case of the presence of NO_3^- ions in the clusters does N_{el} reach the value corresponding to the number of electrons that are active with respect to the radiation in the $(H_2O)_{50}$ cluster. A 2.2-fold larger value of N_{el} has been obtained for the addition of six NO_3^- ions than for the adsorption of six NH_3 molecules. The complex behavior of the $N_{el}(i)$ function suggests that the electronic structure of the entire cluster is changed as a result of adsorption of each NH_3 molecule (or NO_3^- ion). In other words, the adsorption process appears to be electron-sensitive and essentially nonlinear.

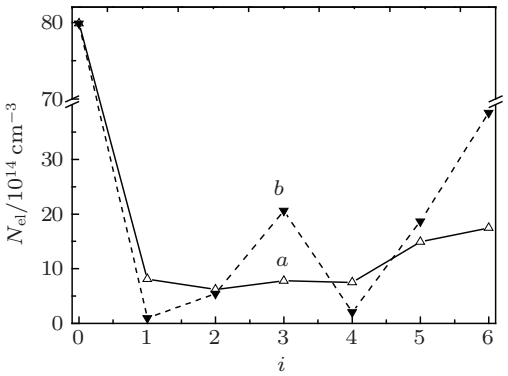


Fig. 5. Densities of electrons interacting with IR radiation for different clusters: $(NH_3)_i(H_2O)_{50}$ (curve a) and $(NO_3)_i^-(H_2O)_{50}$ (curve b), $i = 1, \ldots, 6$.

5. Conclusion

The performed simulation has shown that NH_3 molecules occurring near the surface of a water cluster are absorbed by the latter. As a result, stable $(NH_3)_i(H_2O)_{50}$ clusters containing 1–6 ammonia molecules have been obtained. Due to the internal flexibility of molecules, local structural distortions related to the adsorption of NH_3 molecules by water clusters are minimized. The system of water–ammonia clusters exhibits more intense IR absorption spectra and less intense emission and reflection spectra than does the system of pure water clusters. Moreover, after ammonia molecules are adsorbed, the reflection spectrum exchanges its continuous shape for a banded one. Upon the addition of ammonia molecules to water clusters, a noticeable reduction has been observed in the number of electrons that are active with respect to electromagnetic radiation, with subsequent addition of these molecules causing a complex sign-changing variation in the $N_{el}(i)$ function.

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