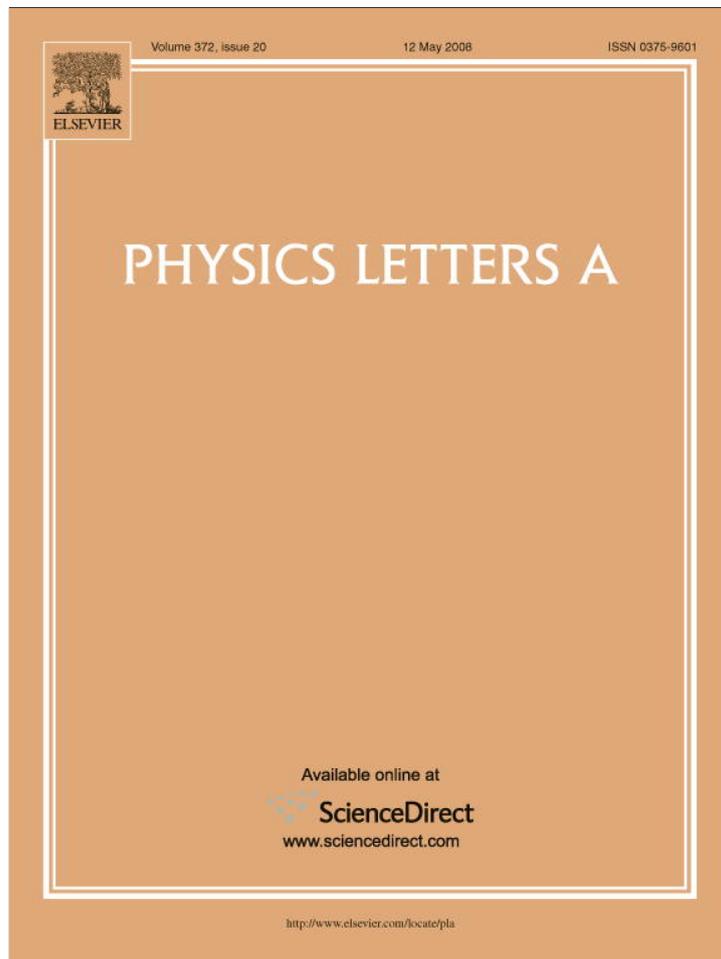


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Computer study of acetylene and ethane adsorption by disperse water medium

A.Y. Galashev*, O.R. Rakhmanova

Institute of Industrial Ecology of the Ural Branch of the Russian Academy of Sciences, S. Kovalevskaya St., 20a, 620219 Yekaterinburg, Russia

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Abstract

Adsorption of acetylene and ethane molecules by water clusters has been investigated by the molecular dynamics method at $T = 233$ K. With the help of determination of statistical weights the cluster systems are created. In the frequency range of $0 \leq \omega \leq 1000$ cm^{-1} the integral absorption coefficient of IR-radiation increases after the adsorption of acetylene or ethane molecules by the ultra disperse water system. The dissipation power of IR-radiation by cluster systems increases if C_2H_2 molecules are adsorbed, and it reduces in the case of C_2H_6 molecules' adsorption. © 2008 Elsevier B.V. All rights reserved.

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Keywords: Water clusters; Acetylene; Absorption coefficient; IR-radiation

1. Introduction

The multiscale is an internal property inherent for water, i.e., water displays various roles on various scales [1]. For example, at the dissolution of biomolecules in water it is important that they are surrounded by water molecules situated at short distances and creating short-range hydrogen linking with them. The display of “hydrophobic” effect requires the longer organization of a system on the longer scales. “Hydrophobic” effect is shown at the solution of acetylene and ethane in water. As the substance is poorly soluble in water, acetylene should be kept on the surface of a water system [2]. The best coupling of a linear molecule with a water cluster is reached when the axis of a molecule is directed on a tangent to a cluster surface. There is the analogy with the acetylene adsorption on KCl (100) surface [3]. Ab initio calculations have shown that the most energetically favorable place of C_2H_2 molecules on a silicon surface is formed through the bridge structure [4]. In this

case C atoms of C_2H_2 molecule are “attached” to the surface with a help of Si–H bonds and they are situated opposite with the same Si_2 dimer. It is experimentally shown that among the saturated hydrocarbons, ethane has the lowest free energy of hydration [5]. Hydrogen bonds between two water molecules in solvate ethane layers are stronger than H-bonds in the volume of a water system [6]. Owing to the polarizability of molecules the hydrogen bonds strengthen one to another, i.e., H-bonds between water molecules become stronger due to the electrostatic induction going from the solvate layer.

In the Earth's troposphere precipitation is formed due to which water rotation is carried out. Most atmospheric water is in ultra disperse condition, i.e., as clusters. Water clusters are capable of absorbing molecules of atmospheric gases [7,8] including greenhouse gases [9,10]. The cluster formation and capture of greenhouse gases by water clusters has an influence on the greenhouse effect [11]. Adsorption of molecules of organic compounds by water clusters still remains a poorly studied phenomenon. At the investigation of small water systems, such as clusters, it is necessary to consider the formation of hydrogen bonds between the nearest neighbors. Results of the analysis of IR-spectrum's far region and the calculations

* Corresponding author. Tel.: +7 343 362 32 67.

E-mail address: galashev@ecko.uran.ru (A.Y. Galashev).

executed by the functional density method show the formation of benzene-water dimmers [12] and $C_6H_6(H_2O)_9$ clusters [13] in a cooled supersonic jet. Energy of H-bond in a benzene-water dimer is estimated as 1.9 kcal/mol. Interaction of benzene ring with $(H_2O)_9$ cluster results in formation of one H-bond and in significant change of distances between oxygen atoms (and r_{OH} distances, where O and H atoms belong to different molecules) in cluster. Adsorption of C_2H_2 and C_2H_6 molecules should also result in significant reorganization of all water cluster's structure. It will be shown in turn in the appreciable change of spectral characteristics of ultra disperse water system. Frequency of translation vibrations of three-atomic molecules (in the condensed state) is usually limited, i.e. $\omega < 1000 \text{ cm}^{-1}$ [14]. As a rule, the greater frequencies correspond to the intramolecular vibrations. Near infrared adsorption by water dimmers in the atmosphere was registered in work [15], and in work [16] it was confirmed in laboratory conditions. In the present work the interaction of ultra disperse water medium with hydrocarbon molecules in close to atmospheric conditions is investigated by the molecular dynamics method (MD).

The purpose of the present work is to study the adsorption of acetylene and ethane molecules by water clusters, as well as to determine the influence of these hydrocarbonic molecules on the form of absorption IR-spectra of disperse water medium and to establish a role of C_2H_2 and C_2H_6 molecules in the dissipation of energy of the external IR-radiation acquired by water clusters.

2. Computer model

Water–water interaction was realized using the advanced TIP4P potential, and H_2O molecule was represented by rigid four-centered model [17]. Calculation of the induced dipole moments allowed to take into account the effect of molecules' polarization. The description of hydrocarbon molecules' interaction with water and also between themselves was based on an atom–atom potential calculated in the Gordon–Kim approximation with the application of spherical average of electronic densities [18,19].

Firstly, in the molecular dynamic calculation by the duration of $2 \times 10^6 \Delta t$ an equilibrium condition at $T = 233 \text{ K}$ for water clusters not containing admixture molecules was reached. The configuration of water cluster referring to the moment of time 20 ps was then used as the initial configuration for modeling of the $(C_2H_2)_i(H_2O)_n$ and $(C_2H_6)_i(H_2O)_n$ systems. The C–C axes of attached C_2H_2 and C_2H_6 molecules were firstly orientated in to the direction of the cluster's centre of mass and the least distance between the atoms in admixture molecules and the atoms of water molecules was made of 0.6–0.7 nm. The cut off radius of all interactions in the model was equal 0.9 nm. The equilibration of the newly formed system was carried out within a time interval of $0.6 \times 10^6 \Delta t$ and then in the interval of $2.5 \times 10^6 \Delta t$ the necessary physical and chemical properties were calculated.

We consider some types of ultra disperse systems: $(C_2H_2)_j(H_2O)_n$, $(C_2H_6)_j(H_2O)_n$, $(C_2H_2)_i(H_2O)_{20}$, $(C_2H_6)_i(H_2O)_{20}$, $j = 1, 2$, $10 \leq n \leq 20$, $1 \leq i \leq 6$. It was as-

sumed that cluster containing $i(j)$ admixture molecules and n water molecules has the statistical weight

$$W_{i(j)n} = \frac{N_{i(j)n}}{N_{i(j)\Sigma}}, \quad i = 1, \dots, 6, \quad j = 1, 2, \quad n = 10, \dots, 20,$$

where $N_{i(j)\Sigma} = \sum_{n=10(1)}^{20(6)} N_{i(j)n}$ is the number of clusters with $i(j)$ admixture molecules and n water molecules in 1 cm^3 . The $N_{i(j)\Sigma}$ quantity was estimated as follows. Let us consider the case of non-polarized light's dispersion, where the length of the molecules' run l is much less than the λ length of the light wave. The coefficient of the extinction (weakening) h of a falling beam on the one hand is defined by the Rayleigh [20] formula, and on the other hand is defined through a scattering coefficient ρ ($h = \frac{16\pi}{3}\rho$) [21] in the approximation of scattering at a 90° angle. Considering that $h = \alpha + \rho$, where α is an absorption coefficient, we have

$$N_{i(j)\Sigma} = \frac{2\omega^4 (\sqrt{\epsilon} - 1)^2}{3\pi c^4 \alpha} \left(1 - \frac{3}{16\pi}\right),$$

where c is the light speed, ϵ is the dielectric permittivity of the medium, ω is the frequency of the falling wave. Calculation of all spectral characteristics was carried out subject to the accepted statistical weights $W_{i(j)n}$. The procedure of cluster systems' formation supposes the uniform distribution of these formations and it is justified at the low clusters' concentration, due to this they do not interact among themselves. The average value of each type of clusters' concentration in the investigated systems is less than a Loschmidt number by 12–13 orders.

Absorption of electromagnetic waves of the certain frequency by a molecule can occur only in the case if the molecule's dipole moment makes vibrations with the same frequency. The absorption coefficient is proportional to the square vibration amplitude of the dipole moment. Absorption of radiation on ω frequency at thermodynamic equilibrium in the gas phase with temperature T is characterized by the α absorption coefficient. On the basis of calculation of the autocorrelation function of the d_{cl} cluster's total dipole moment a $\epsilon(\omega)$ complex dielectric permittivity of disperse system dependent on the frequency [22] was determined. The α quantity was represented through the imaginary part of $\epsilon(\omega)$ frequency-dependent dielectric permittivity in the form

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

The $P(\omega)$ frequency dependence of dielectric losses was represented [21] as

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

where $\langle E^2 \rangle$ is an average value of square of the electric field strength, ω is the frequency of emitting electromagnetic wave.

3. The results of calculations

Configurations of $(C_2H_2)_6(H_2O)_{20}$ (a) and $(C_2H_6)_6(H_2O)_{20}$ (b) clusters obtained to the moment of time 25 ps show the absence of stirring of H_2O molecules with C_2H_2 and C_2H_6 molecules even when the number of admixture molecules reaches

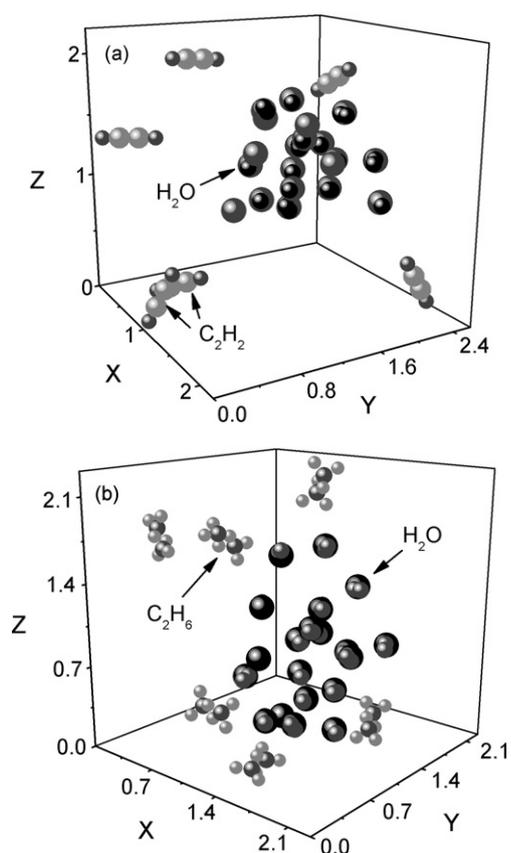


Fig. 1. Configuration of $(\text{C}_2\text{H}_2)_6(\text{H}_2\text{O})_{20}$ (a) $(\text{C}_2\text{H}_6)_6(\text{H}_2\text{O})_{20}$ (b) cluster, corresponding to the moment of time 25 ps. Coordinates of molecules are represented in nm.

six (Fig. 1). Acetylene molecules are attracted by water clusters. Finally, they get the orientation of a tangent to the $(\text{H}_2\text{O})_{20}$ cluster surface. It is reached due to the attraction of C atoms to H atoms of water molecules oriented mainly outward to the cluster. Thus H atoms which are on the ends of C_2H_2 molecule fell the repulsion from the surface of water cluster. In this case acetylene molecules act as proton acceptors [23]. And bond energy with water clusters is estimated as -3.3 , -3.7 and -3.1 kcal/mol for systems $\text{C}_2\text{H}_2(\text{H}_2\text{O})_n$, $(\text{C}_2\text{H}_2)_2(\text{H}_2\text{O})_n$ and $(\text{C}_2\text{H}_2)_i(\text{H}_2\text{O})_{20}$ accordingly. These values are coordinated with the estimation of bond energy (-3.7 kcal/mol) for the acetylene acting as a proton acceptor to amorphous ice [24]. For acetylene–water dimer the bond energy is determined at $-(1.2\text{--}1.9)$ kcal/mol (acetylene–proton acceptor) and $-(2.1\text{--}3.2)$ kcal/mol (acetylene–proton donor) [25]. Interaction of ethane molecules with water clusters is characterized by higher values of bond energy. For systems of $\text{C}_2\text{H}_6(\text{H}_2\text{O})_n$, $(\text{C}_2\text{H}_6)_2(\text{H}_2\text{O})_n$ and $(\text{C}_2\text{H}_6)_i(\text{H}_2\text{O})_{20}$ these values are equal -2.8 , -2.8 and -1.6 kcal/mol accordingly. If in general for the two first systems the ethane acts as proton acceptor then for the last system it acts in a role of proton donor (oxygen–hydrogen of ethane pairs give the lowest energy in the ethane–water interaction). Thus, with the growth of ethane concentration and the amplification of interaction between C_2H_6 molecules the switching of the bond type from proton acceptor to proton donor is observed. Bond energy in a complex amorphous ice–

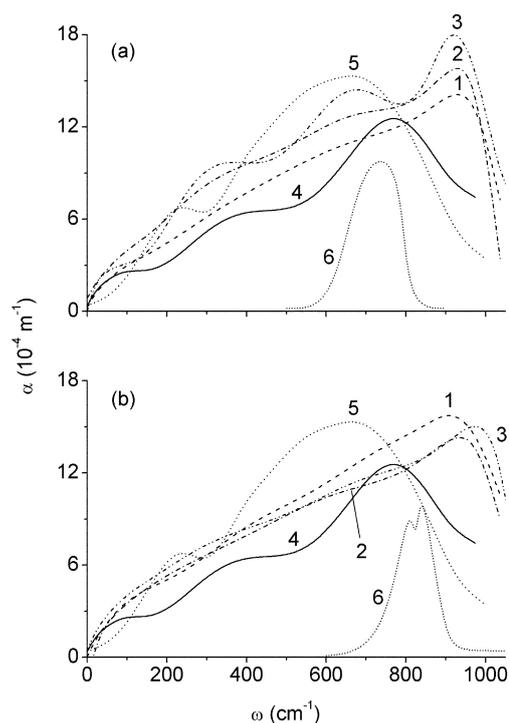


Fig. 2. Absorption coefficient of IR radiation for cluster systems: (a): 1— $\text{C}_2\text{H}_2(\text{H}_2\text{O})_n$, 2— $(\text{C}_2\text{H}_2)_2(\text{H}_2\text{O})_n$, 3— $(\text{C}_2\text{H}_2)_i(\text{H}_2\text{O})_{20}$, (b): 1— $\text{C}_2\text{H}_6(\text{H}_2\text{O})_n$, 2— $(\text{C}_2\text{H}_6)_2(\text{H}_2\text{O})_n$, 3— $(\text{C}_2\text{H}_6)_i(\text{H}_2\text{O})_{20}$; 4— $(\text{H}_2\text{O})_n$, 5— $\alpha_w(\omega)$ function of bulk water, experiment [26], 6—experimental spectrum for gaseous hydrocarbon: (a)— C_2H_2 , (b)— C_2H_6 [27].

ethylene (proton acceptor) is estimated as -3.8 kcal/mol [24]. At atmospheric pressure the ethylene has the higher solubility in water than ethane. The C_2H_6 molecules are not rejected by water cluster but also do not approach it too close being symmetrically on opposite sides of the cluster.

The frequency dependence of $\alpha(\omega)$ IR-radiation absorption coefficient of investigated systems is shown in Fig. 2. The $\alpha(\omega)$ coefficient for disperse systems containing C_2H_2 molecules is higher than for the disperse system of pure water (Fig. 2(a)). The intensity of spectrum is increased with the growth of C_2H_2 molecules' number in the water system. The principal maximum of $\alpha(\omega)$ distribution for the system of pure disperse water falls to the frequency of 780 cm^{-1} and for the similar water system with one and two acetylene molecules in each cluster is at 970 cm^{-1} . After absorption from one up to six acetylene molecules by monodisperse water system the $\alpha(\omega)$ spectrum becomes strongly oscillating with the principal maximum at $\omega = 920\text{ cm}^{-1}$. The $\alpha_w(\omega)$ spectrum of bulk liquid water [26] has two maxima at frequencies of $\omega = 200$ and 700 cm^{-1} . The higher integrated intensity of IR radiation absorption for bulk water is caused by its density which is higher, on average, than the density of water clusters by a factor of 1.4. However, at the presence of hydrocarbon molecules in these clusters the density is not a determining factor in the absorption of IR radiation. The expansion of system owing to the attachment of hydrocarbon molecules results in an increase of the number of vibration modes including the $0 \leq \omega \leq 1000\text{ cm}^{-1}$ frequency range of $\alpha(\omega)$ spectrum. Orientation of acetylene molecules

on a tangent to water cluster gives a stable amplification of the integrated intensity of $\alpha(\omega)$ spectrum with the growth of acetylene concentration. This is promoted by repulsion of positive charges of C_2H_2 molecules. The bending band of $\alpha(\omega)$ spectrum of gaseous acetylene is located at the frequency of $\omega = 730\text{ cm}^{-1}$ [27]. Thus attachment of acetylene molecules by water clusters strengthens the integrated I_{tot} absorption intensity.

The more chaotic orientation of ethane molecules in clusters causes a less stable change of the vibrations' intensity with the growth of the number of C_2H_6 molecules that is reflected in the behavior of the IR spectrum absorption. After adsorption of one ethane molecule the absorption of external IR-radiation in the investigated frequency range by ultra disperse water systems is also amplified (Fig. 2(b)) and the form of the curve becomes smoother. However, the following addition of C_2H_6 molecules results in some decrease of the IR-radiation absorption, at least at frequencies of $\omega > 310\text{ cm}^{-1}$. Nevertheless, almost in all frequency range (except for the area of $690 \leq \omega \leq 800\text{ cm}^{-1}$) the values of α coefficient for the systems consisting of heteroclusters are higher than for a cluster system of pure water. The principal maximum of $\alpha(\omega)$ frequency spectrum appears at $\omega = 910\text{ cm}^{-1}$ ($C_2H_6(H_2O)_n$ system) and $\omega = 973\text{ cm}^{-1}$ ($(C_2H_6)_2(H_2O)_n$ and $(C_2H_6)_i(H_2O)_{20}$ systems). The part of $\alpha(\omega)$ spectrum determined by the bending vibrations of gaseous ethane's molecules has the doubled maximum in $810 \leq \omega \leq 840\text{ cm}^{-1}$ frequency range [27].

Water clusters including clusters absorbing acetylene or ethane molecules are capable to re-emit of the falling IR-radiation. Calculations show that disperse system consisting of pure water clusters has low values of P radiation power, in comparison with the system enriched with acetylene (Fig. 3(a)). For the disperse system formed by pure water, two characteristic frequencies of IR-radiation are observed: $\omega_1 = 657\text{ cm}^{-1}$ and $\omega_2 = 973\text{ cm}^{-1}$. The maximal value of emitted radiation power corresponds to the frequency of 970 cm^{-1} when only one C_2H_2 molecule is present in clusters, and to the frequency of 910 cm^{-1} at the presence of two acetylene molecules in every cluster of the system. After adsorption of the second C_2H_2 molecule by clusters the radiation power of disperse systems is increased. And the adsorption of ethane molecules by water clusters causes the essential decrease of clusters' P radiation power (Fig. 3(b), on an insert). Arrangement of C_2H_2 molecules on a tangent to a surface of water clusters makes their structure more dense [28]. Due to C atoms the acetylene molecule is attached to the cluster. Due to H atoms the molecule keeps a tangent direction to the water cluster and makes it denser. As a rule \bar{n}_b , an average number of hydrogen bonds per molecule decreases, and \bar{L}_b , the H-bond length, increases during the addition of both acetylene and ethane molecules to water clusters [28,29]. When the number of admixture molecules $i < 5$, the value of \bar{n}_b for water clusters with C_2H_2 molecules is higher and \bar{L}_b is lower, than for clusters with C_2H_6 molecules. The volume of water clusters with C_2H_2 molecules appears to be 5–10% less than the volume of similar clusters with C_2H_6 molecules. As a result, the D_w self-diffusion coefficient of water molecules in $(C_2H_2)_i(H_2O)_j$ clusters is on average 20–30%

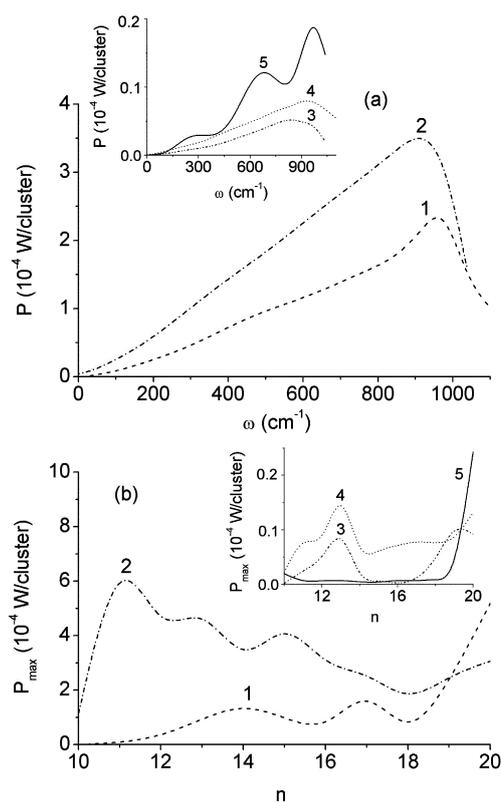


Fig. 3. Frequency dependence of $P(\omega)$ IR radiation power (a) and dependence of maximum P quantity on n number of water molecules in clusters (b): 1— $C_2H_2(H_2O)_n$, 2— $(C_2H_2)_2(H_2O)_n$, 3— $C_2H_6(H_2O)_n$, 4— $(C_2H_6)_2(H_2O)_n$, 5— $(H_2O)_n$.

lower than in $(C_2H_6)_i(H_2O)_j$ clusters. The D_a self-diffusion coefficient of C_2H_2 molecules is higher than D_a value for C_2H_6 molecules by no more than 1%. The decrease of D_w value causes the amplification of collective vibrations that, in turn, causes an appreciable amplification of dissipation of absorbed energy. An average \bar{d}_{cl} dipole moment of $(C_2H_2)_i(H_2O)_j$ clusters exceeds the appropriate \bar{d}_{cl} value of $(C_2H_6)_i(H_2O)_j$ clusters on an average by 5%. The ϵ'' imaginary part of dielectric permittivity of $(C_2H_2)_i(H_2O)_j$ clusters can increase by an order in comparison with the ϵ'' value of pure water clusters. This causes a sharp amplification of emitted radiation power for the system formed from these clusters. For $(C_2H_6)_i(H_2O)_j$ clusters the opposite picture is observed, i.e. the ϵ'' value significantly reduces (up to 5 times) which causes an appreciable easing of the power of emitted IR radiation by an appropriate cluster system. The $P(\omega)$ spectra for the systems consisting of heteroclusters become smoother than for clusters system of pure water. The doubling of C_2H_6 molecules' number in ultra disperse system results in some amplification of radiation power. The principal maxima of $P(\omega)$ spectra for the systems containing one and two ethane molecules in clusters are located at $\omega = 847$ and 910 cm^{-1} accordingly.

The behavior of P_{max} maximal value of clusters in dependence on a number of water molecules containing in clusters is shown in Fig. 3(b). Pure water clusters are characterized by an extremely low rate of energy dissipation up to the size $n = 18$ (an insert in Fig. 3(b)). For $(H_2O)_n$ clusters with $n > 18$ the

radiation power is sharply increased, but still remains enough low in comparison with the similar characteristic of clusters containing C_2H_2 molecules. The maximal values of the radiation power of water clusters adding one C_2H_2 molecule up to the size $n = 18$ is considerably lower than the P_{max} quantity of $(C_2H_2)_2(H_2O)_n$ clusters. Almost everywhere the P_{max} values for clusters of system where each aggregate contains two ethane molecules exceed the appropriate characteristics of aggregates of system with one C_2H_6 molecule. At the same time clusters containing ethane molecules, as a rule, have the higher P_{max} values than pure water clusters. Water clusters with $n = 10, 16$ and 20 are an exception here.

4. Conclusion

Results of molecular dynamic calculation of hydrocarbons molecules' adsorption by ultra disperse water medium show that acetylene molecules are at a tangent to the water core of the $(C_2H_2)_i(H_2O)_n$ clusters. While in $(C_2H_6)_i(H_2O)_n$ clusters each C_2H_6 molecule is directed to the water core of aggregate arbitrarily, i.e., its C–C axis is not directed to the cluster's centre of the mass and does not have tangent direction to the aggregate's core. Adding of one acetylene or ethane molecule is accompanied by the increase of IR-radiation absorption coefficient of disperse systems. However during the further increase of admixture molecules' concentration in water clusters the α coefficient grows in the case of addition of C_2H_2 molecules, and decreases at the adsorption of C_2H_6 molecules. Also after adding C_2H_2 or C_2H_6 molecules by disperse water systems the frequency corresponding to the maximum of IR-radiation absorption is also increased. Adsorption of acetylene molecules by water clusters results in a significant amplification of the radiation power by cluster systems. Thus the dissipation rate of acquired energy grows with the increase of C_2H_2 molecules' concentration in the system. Clusters with 20 water molecules not containing or containing only one C_2H_2 molecule and cluster with 11 H_2O molecules capturing two C_2H_2 molecules have the highest radiation power. On the contrary, ultra disperse system made up of water clusters enriched with ethane molecules loses the emitting power of heat. But with the growth of ethane concentration the IR-radiation power is amplified and the maximum of emitting power is shifted from $n = 19$ to $n = 13$.

As a whole clusterization and adsorption of hydrocarbons molecules by clusters results in a decrease of the greenhouse effect because of the decrease of absorption centers' number of IR-radiation and the insufficient amplification of its integral intensity caused by the adsorption of C_2H_2 and C_2H_6 molecules.

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