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Theoretical study of ir stretching bands of water molecules and their deuterated analogues in complexes with triacetin using density functional theory methods

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In this work, a theoretical investigation of the IR stretching bands of water molecules and their deuterated analogues in complexes with triacetin was carried out using density functional theory (DFT) methods. Molecular models of a triacetin dimer with different types of hydrogen bonds single and double as well as water clusters were constructed. Thermodynamic parameters of complex association, including enthalpy and equilibrium constants, were calculated with consideration of basis set superposition error. Model IR absorption bands were generated using Gaussian profiles that account for Fermi resonance and show good agreement with experimental data. It was established that the complex with a single hydrogen bond is energetically more stable than the one with a double bond, and that the presence of a water bridge affects the association parameters for the addition of a second water molecule. The results support experimental observations on the structure and dynamics of hydrogen bonding in triglyceride water systems, contributing to the understanding of fat hydration.

Keywords: triglycerides, hydrogen bonding, density functional theory, fat hydration, association thermodynamics, IR spectroscopy.

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Introduction

Triglycerides, as the main components of fats and oils, are esters of glycerol and three chains of fatty acids that play a key role in various scientific and industrial fields, including food industry, energy and pharmaceuticals [1–3]. Their interactions with water molecules determine the properties of systems, such as emulsions, lipid carriers, and biological membranes, where the hydrophobicity of triglycerides limits solubility in water, but molecules can orient themselves at the interface to minimize interfacial energy [4–6].

Molecular modeling, including molecular dynamics, shows that at the boundary with water, triglycerides position the glycerol fragment towards the aqueous phase, facilitating penetration of water through interactions with oxygen atoms of ester groups [3]. Such orientations stabilize the water-organic interfaces which is critical for the emulsion [7]. In addition, the presence of water in the triglyceride matrix affects the solubility of small molecules, which is important for lipid drug delivery systems. In complex products such as butter, fat-water boundaries limit the diffusion of flavors, emphasizing the complex organization of the interface [9].

Experimental methods such as 2D-IR-spectroscopy reveal that water in triglyceride oils stabilizes as monomers or clusters, forming strong single hydrogen bonds (HB) with carbonyl groups and weak double bonds, possibly in the form of „bridges“ between neighboring molecules [10]. Yet, the molecular pattern of these interactions remains not fully clear. Quantum chemical studies, including theory of the density functional, allow to analyze in detail the hydrolysis and methanolysis of triglycerides such as triacetin, modeling energy barriers and the role of HB in reactions with water [11,12]. Similarly, the analysis by the theory of the density functional of water IR-spectra at interfaces with hydrophobic polymers confirm the HB configurations, where OH-strains decompose into components depending on the strength of the bonds [13].

Despite the progress, the mechanisms of triglyceride hydration, the effect of unsaturation and chain length of fatty acids on HB require further study. Modern methods of molecular dynamics and quantum chemistry provide tools for atomic-level analysis of these processes.

The purpose of this study is a theoretical explanation of the experimentally registered IR bands of valence vibrations of water molecules and their deuterium analogues forming

HB with triacetin jcite10. For this purpose, molecular models of triacetin dimer complexes with water molecules were constructed and studied using density functional theory methods.

1. Calculation procedure

The quantum chemical analysis was made using Gaussian software package [14]. The geometry was improved and vibrational spectra were analyzed using the hybrid functional B3LYP [15,16] and basic set of Gaussian functions 6-31+G(d) [17–19]. In order to ensure high accuracy and convergence of calculations, the geometry improvement, self-consistent field calculation and integration were performed with strict criteria: opt = tight, SCF = Tight and Int = UltraFine, respectively. After calculation, the wave numbers were refined using the linear scaling method [20–22] according to the empirical ratio

$$\omega_{\text{exp}}/\omega_{theor} = a\omega_{theor} + b, \qquad (1)$$

where ω_{exp} and ω_{theor} — experimental and calculated wavenumbers, [cm^{-1}], a and b — coefficients to be found. For the basis 6-31+G(d) $a = -8.71 \cdot 10^{-6}$, $b = 0.9863$.

The complexes association enthalpy was found using the hybrid calculation scheme. Geometric parameters and wave numbers were calculated using B3LYP/6-31+G(d) method, and the electronic energy was refined using a single self-consistent field procedure using wB97XD [23] functional with the extended basis set 6-311+G(d, p). For this basis the basis set superposition error (BSSE) was found [24]. The enthalpy was found by formula

$$\Delta H_T^0 = \Delta E + \Delta ZPE + \text{BSSE} + \Delta H_{term}, \qquad (2)$$

where ΔE — the difference of the total electronic energies of the dimer and monomers, ΔZPE — the difference of zero vibrational energies, BSSE — superposition error, ΔH_{term} — thermodynamic correction, which was found by formulas [25].

2. Building molecular models

Triglycerides of fatty acids have high mobility, which leads to the formation of many conformations with minor energy differences comparable to RT (R — universal gas constant, T — absolute temperature). Triacetin is the simplest triglyceride of acetic acid and has 109 different conformers, of which more than 30 occur with a probability higher than 1,% [26]. Thus, fats are an equilibrium mixture of many forms of triglycerides similar in energy. In this study, molecular models of triglycerides were used, which are located in one of the possible local minima of potential energy. The same structures were previously used to analyze the spectral properties of vegetable oils [27–29]. In the selected model, the hydrocarbon chains form a „trident“, located in one half-plane, while the two carbonyl groups are located in the other. A similar structure can form at the fat-water interface, when carbonyl groups are oriented towards the aqueous phase to reduce the energy of interaction. In [10], it was found that triacetin forms two types of complexes with a water molecule. One by forming one strong HB with its carbonyl group, and the other by forming two weak HBs presumably with carbonyl groups of two different triacetins. Based on this data, triacetin dimer was taken as a molecular model. The initial structure of dimers was built by direct superposition of two triglycerides. The improved structure of triacetin dimer is shown in Fig 1, *a*.

When building molecular models of triglyceride dimers complexes with water molecules for the case of a double HB, three water molecules were initially added to the improved dimer according to the number of carbonyl groups, followed by improvement. A complex containing three molecules of water was obtained in result. The improved structure of this complex is shown in Fig. 1, *b*. A complex with three different variants of water molecule attachment was obtained: one water molecule forms two HB with the oxides of the ester groups of two different triacetins (K1), the second water molecule forms two HB with the carbonyl group of one triglyceride and with the oxygen of ester group of another (K2), while the third water molecule has two carbonyl groups (K3). Further, an additional analysis of these structures was carried out separately. K1 complex is not separately stabilized but is transformed into K3 complex. K2 and K3 complexes are stabilized and their structure is shown in Fig 1, *c*, *d*.

Analysis of thermodynamic parameters of two complexes K2 and K3 showed that K2 had greater energy stability $\Delta H_T^0 = -19.9$ kJ/mol, compared to K3 $\Delta H_T^0 = -15.9$ kJ/mol. At the same time, the equilibrium constant of K2 complex is 3.2 times less. This is because of high entropy losses of K2 - parameter $T\Delta S = -39.2$ kJ/mol against -32.2 kJ/mol of K3. This suggests that K2 complex has a more rigid structure due to the combination of carbonyl and etheric HB, which restrict the freedom of movement of molecules more strongly compared to the case when both hydrogen bonds are formed with carbonyl groups. Due to the advantageous steric arrangement of carbonyl groups, the probability of forming a complex with them is much higher. In [10], it is mentioned that hydrogen bonds have stable energy, which indicates that there are complexes of a certain type. Based on this, in further modeling, we used K3 complex.

Next, a model of a complex with a single HB was built. A water molecule was added in such a way that a single HB was formed with oxygen of the free carbonyl group of one triglyceride (K4). The structure of K4 complex is shown in Fig. 1, *e*. This model was used to estimate the thermodynamic parameters of the association and the effect of such an attachment on the dimer geometry.

This estimate was made for two cases. The first case is when K3 complex was formed first, and then a water

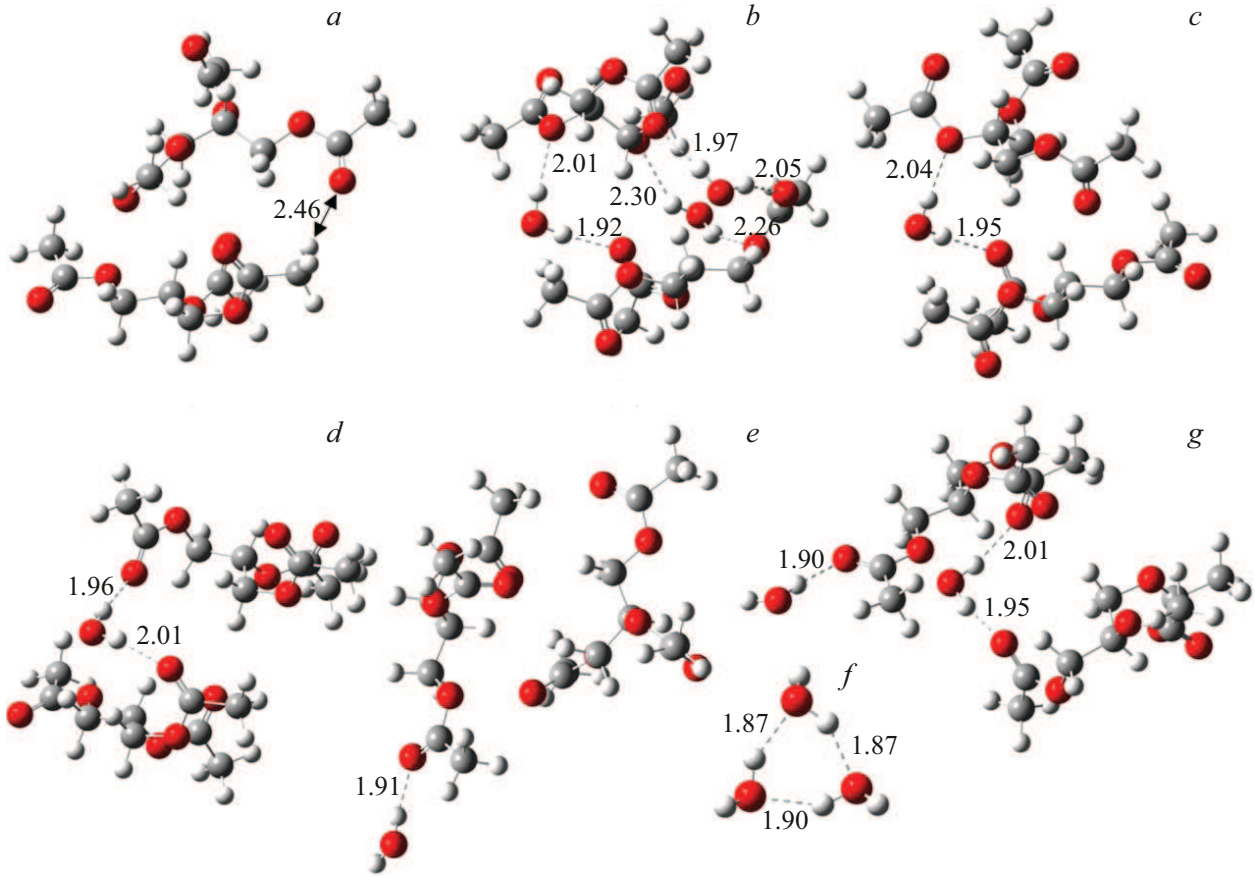

Figure 1. Molecular models of triacetin dimer, its complexes and trimers H_2O improved by method of B3LYP/6-31+G(*d*): *a* — structure of triacetin dimer; *b* — dimer complex with three molecules of H_2O; *c* — K2 complex; *d* — K3 complex; *e* — K4 complex; *f* — structure of a ring trimer H_2O; *g* — K5 complex. The double arrow indicates the minimum distance between the atoms of the two triacetins in the dimer. The hydrogen bonds (HB) are shown by dashed lines, their lengths (in angstroms) are indicated by numbers.

molecule with a single HB was attached to it. In the second case when K4 complex with one HB had a water molecule with two HB attached to it. As a result, a complex containing two water molecules (K5) was obtained, the structure of which is shown in Fig. 1, *g*. This complex was used to model the IR absorption bands of hydrogen-bound water molecules. In [10], it is noted that the presence of water clusters is spectroscopically observed during the interaction of triacetin with water. To model water clusters, the structure of a cyclic water trimer was built (Fig. 1, *f*), for which the Fermi interaction constant [30] is experimentally known. The thermodynamic parameters of the association of triacetin complexes with water molecules are shown in the table below.

The table shows that formation of a complex with a single HB does not noticeably affect the attachment parameters of the second water molecule. The values of the thermodynamic parameters and the equilibrium constant within a given accuracy are the same for K3 complex and $K4 + H_2O$ complex. K4 complex is stronger and more stable than K3. This can be seen by the enthalpy parameters and the equilibrium constant. The enthalpy of formation of two HB in K3 complex correlates with the enthalpy of water dimer [31]. It is possible to confirm the assumption of authors in [10], that one of the water molecules forms a bridge between two carbonyl groups of different triacetin molecules, forming two weak HB.

The absence or presence of an aqueous bridge in the triacetin dimer already significantly affects the parameters of the association to the carbonyl group of one of the water molecule's triacetins. This can be seen from comparing the parameters of K4 and $K3 + H_2O$ in the table. Different values of BSSE make a significant contribution to the difference in parameters, and as a result, in the presence of a bridge, it becomes more advantageous to form a complex with a second water molecule than with a free dimer.

3. Modeling of IR contours

The model IR bands were built using Gaussian contours. The half-widths of the bands for the description were chosen in the same range of values as in [10] when separating the experimental bands. For the band formed by the symmetrical valence vibration of a water molecule

Comparative thermodynamic characteristics of the studied molecular complexes

Complexes	ΔE	BSSE	ΔZPE	ΔH_0^0	ΔH_T^0	$T\Delta S$	K_a
Triacetin dimer	−57.7	4.9	5.6	−47.2	−45.2	−52.6	$5.1 \cdot 10^{-2}$
K3 complex	−29.6	5.2	11.0	−13.3	−15.9	−32.2	$1.4 \cdot 10^{-3}$
Complex K4 + H_2O = K5	−29.6	5.2	11.0	−13.3	−15.9	−32.2	$1.4 \cdot 10^{-3}$
Complex K4	−31.3	3.2	7.7	−20.4	−21.0	−30.9	$1.8 \cdot 10^{-2}$
Complex K3 + H_2O = K5	−31.3	2.0	7.8	−21.7	−22.4	−31.3	$2.8 \cdot 10^{-2}$

Note. Energy parameters: ΔE — energy of complex bond; BSSE — basis set superposition error; ΔZPE — correction for zero vibrations, ΔH_0^0 — change of enthalpy at 0 K; ΔH_T^0 — change of enthalpy at 298.15 K; $T\Delta S$ — contribution of entropy term at 298.15 K, are expressed in kJ·moll^{-1}, K_a — dimensionless equilibrium constant

with one HB 220 cm^{-1}, for the antisymmetric vibration band 38 cm^{-1}, for the overtone band of the deformation vibration 120 cm^{-1}. For the water molecule which forms a bridge of 90, 65 and 100 cm^{-1} respectively; for the water cluster 220, 90, 120 cm^{-1}. Based on the comparison of the values, the half-widths of the experimental absorption bands decreased by 1.25 times during transition to D_2O and HDO molecules. The Fermi interaction constants for H_2O molecules in the complex were selected empirically to reproduce the shape of the experimental band. After that, they were transferred unchanged for modelling the IR band in the complex with D_2O. For water molecule with a single HB the Fermi constant was equal 75 cm^{-1}, with two HB 50 cm^{-1}. The intensity redistribution at Fermi resonance was calculated in the approximation of zero intensity of the strain vibration overtone. When modeling the spectra of HDO molecules, due to the large difference in mass, all the oscillators O-H and O-D are separate and the overtone of the deformation vibration does not interact with the basic tone of the valence vibration O-D. All possible combinations of oscillators O-H and O-D were calculated, four for K5 complex and eight for HDO trimer. The trimer spectrum was plotted from an empirical ratio of 1:15, the number of clusters and the number of K5 complexes. The experimental contours of IR-bands were taken from the study [10] and digitized.

4. Results and discussion

Experimental [10] and theoretical IR bands of the hydrogen-bound HDO molecules in the region of 2300 − 2800 cm^{-1} are illustrated in Fig. 2.

The general shape of the theoretical band is in good agreement with the experimental data. The basis of the band intensity is determined by three fluctuations. The most intensive among them is the vibration of the hydrogen-bound oscillator O-D $\omega_{theor} = 2536$ cm^{-1} of HDO molecule that forms a single HB. The other two bands imposed over each other $\omega_{theor} = 2587$ cm^{-1} and $\omega_{theor} = 2603$ cm^{-1} relate to O-D oscillators of the second HDO molecule. A very weak oscillation band of the unbound oscillator OD $\omega_{theor} = 2663$,cm^{-1} manifests itself only as a very small change in the shape of the lower part of the general contour on the right. The spectrum of water clusters in the form of a wide band $\omega_{theor} = 2472$ cm^{-1} somewhat affects the elevation of the left side of the contour.

Modeling the vibration contours of hydrogen-bound molecules of H_2O and D_2O is more complex than in the first case, since it is necessary to take into account resonant interactions that manifest themselves in the spectra and greatly impact the shape of the absorption bands contours. Experimental and theoretical IR adsorption bands of H_2O in the region 3100−3800 cm^{-1} and of D_2O in the region 2300−2800 cm^{-1} are illustrated in Fig. 3.

Figure 3 shows that Fermi constants found using the density functional method and selected empirically make it possible to well describe the complex shape of the absorption band of H_2O molecules hydrogen-bonded to triacetin. All vibrations of water molecules in this region are significantly involved in the formation of the band, starting from the highest frequency antisymmetric vibrations $\omega_{theor} = 3647$ cm^{-1} of a water molecule on one side, to the lowest frequency overtone $\omega_{theor} = 3259$ cm^{-1} of the deformation vibrations of the same water molecule. As can be seen by comparing the theoretical and experimental spectra, the highest frequency vibration goes beyond the contour of the antisymmetric vibration $\omega_{theor} = 3259$ cm^{-1} of the second water molecule, which creates distortions on the right side of the contour. This is because of a limitation of our molecular model, which does not provide for the van der Waals interaction of an unbound hydrogen atom with its environment, which would lead to a slight shift of this band to the left. Apart from this case, the remaining individual bands correspond in relative position to the separated bands based on the experimental contour.

When transferring to a complex with D_2O molecules the situation becomes somewhat worse. In addition to a similar problem with the antisymmetric vibration $\omega_{theor} = 2690$ cm^{-1}, there is a relatively overestimated intensity of the symmetrical vibration $\omega_{theor} = 2569$ cm^{-1} of D_2O molecule, which is a bridge. Because of this, the contour shape is distorted compared to the experimental

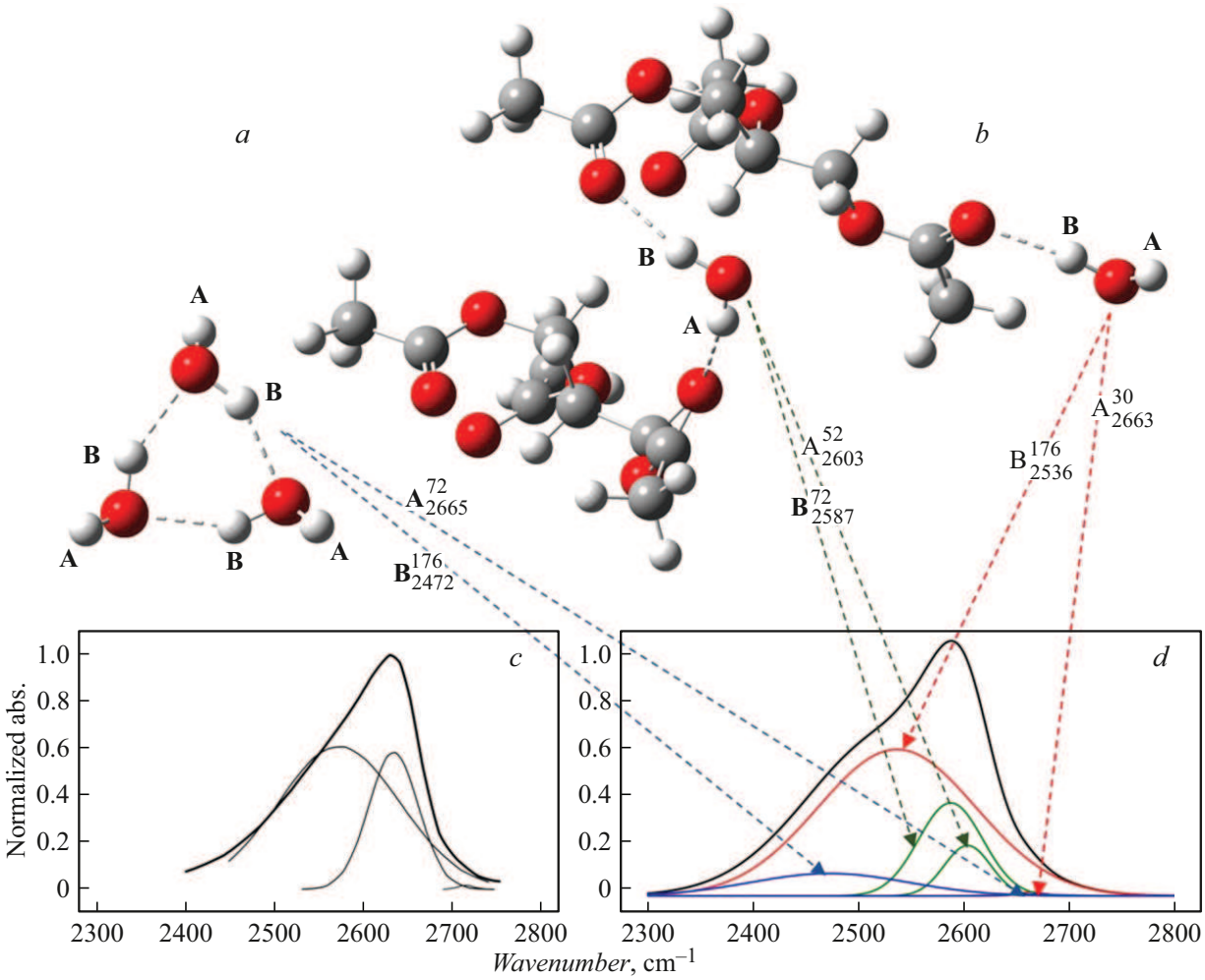

Figure 2. Molecular models of water cluster (*a*) and complex of triacetin dimer with two molecules of HDO (*b*), improved by method B3LYP/6-31+G(*d*). Experimental [10] IR-band of HDO molecules absorption (*b*) bound together with triacetin molecules (possible contours of individual absorption bands are shown inside the main contour). Spectral model of the absorption band of HDO (*d*) molecules in a complex with a triacetin dimer together with the corresponding cluster $(HDO)_3$. The dashed line shows hydrogen bonds. The dashed arrows indicate individual adsorption bands corresponding to different types of oscillators: *A* — oscillator O-D(A), *B* — oscillator O-D(*B*). The upper index shows the half-width of the model band, and the lower index shows the maximum position of the band in units, [cm^{-1}].

one. Despite this, the qualitative description of the shape of this strip can be considered satisfactory.

Conclusion

The study made it possible to explain the experimentally observed shapes of IR bands of water molecules valence vibrations and their deuterium analogues in complexes with triacetin. Molecular models of the triacetin dimer with various HB configurations (single and double), as well as cyclic water trimer, were built and analyzed using methods of density functional theory. Calculations have shown that K4 single hydrogen bond complex has greater energy stability ($\Delta H_T^0 = -21.0$ kJ/mol) compared to K3 double bond complex ($\Delta H_T^0 = -15.9$ kJ/mol). The model IR bands built given the Fermi resonance and empirically selected interaction constants demonstrate a qualitative consistency with the experimental spectra in $2300-3800\,cm^{-1}$ region. The most significant contribution to the bands' intensity comes from symmetrical vibration of single hydrogen-bound oscillators of O-Dand O-H molecules with a single HB, while high-frequency antisymmetric vibrations require to allow for the van der Waals interactions. The results obtained confirm experimental data and assumptions about the structure of hydrogen bonds and their role in triglyceride hydration and emphasize the importance of taking into account water bridges and clusters when modeling the spectral and thermodynamic properties of such systems. The study contributes to the development of molecular modeling of lipid-water interfaces, which is important for biochemistry, pharmaceuticals and the food industry.

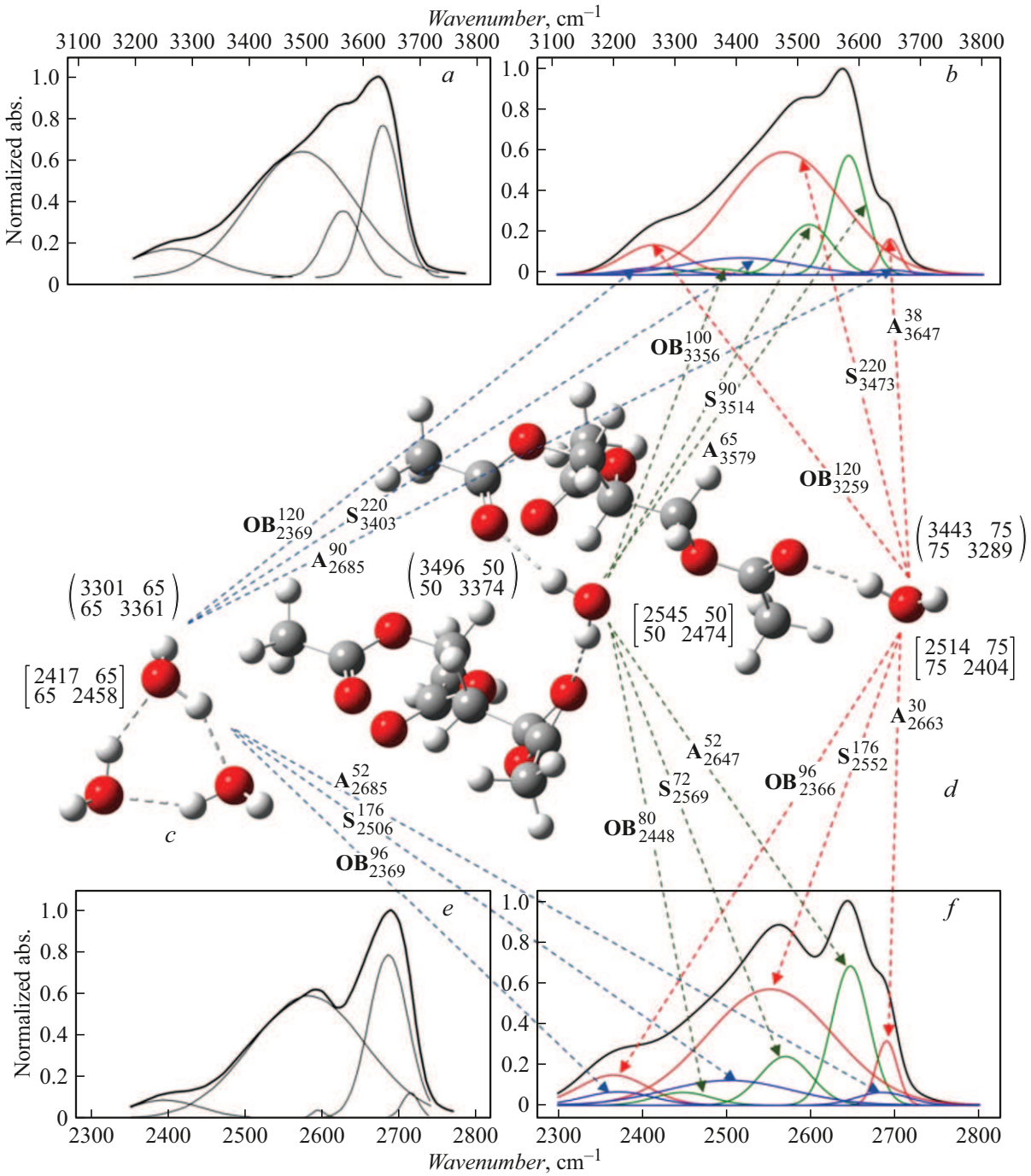

Figure 3. Experimental [10] IR absorption bands of H_2O (*a*) and D_2O (*e*) molecules bound with triacetin molecules via hydrogen bonds (possible contours of individual absorption bands are shown inside the main contour). Molecular models of an aqueous cluster (*c*) and triacetin dimer complex with two molecules of water (*d*) improved by method B3LYP/6-31+G(*d*). Spectral models of H_2O (*b*) and D_2O (*f*) molecules adsorption bands in a complex with triacetin dimer together with appropriate clusters $(H_2O)_3$ and $(D_2O)_3$. The dashed line shows hydrogen bonds. The dashed arrows indicate individual absorption bands corresponding to different types of vibrations: A — antisymmetric valence vibrations of O-H and O-D bonds, S — symmetric valence vibrations, OB — overtone of deformation vibration. The upper index shows the half-width of the model band, and the lower one shows maximum position of the band in units[cm^{-1}]. The values in parentheses designate the parameters of Fermi resonators in units, [cm^{-1}] for H_2O molecules, while the values in brackets designate the parameters for D_2O molecules.

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Conflict of interest

The authors declare that they have no conflict of interest.

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