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## VIRTUAL WATER MOLECULE DISSOCIATION IN EXTERNAL ELECTROMAGNETIC FIELDS

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The model is proposed for describing a real water molecule by its two-dimensional analog, namely, the virtual molecule (VM). The proposed VM model provides the condition of coincidence between the fundamental eigenfrequencies of the real molecule and its virtual analog. The other VM parameters (bond length and atomic mass) are renormalized so that the molecule should steadily exist for a long time interval. Linear dynamics of VM atoms in the field of a monochromatic electromagnetic wave has been investigated. It is shown that under the action of an external electromagnetic field on the molecule at a resonance frequency, secular modes of vibrations are observed. The last ones are characterized by a time-linear growth of atomic oscillation amplitudes. The influence of the turn on of an external force at the time of stabilization of eigenfrequencies of the VM on the stability of VM atomic oscillations were made. It is shown that in some cases breaking of one of the VM bonds inevitably leads to the VM dissociation as a whole. As a result of numerical simulation, it has been established that the bond breaking has a threshold character, i.e., dissociation is not observed at the external force, which is below a certain value. In the region of forces exceeding the threshold values, the variation in the external electromagnetic field frequency is insensitive to the resonance effects that are due to the presence of dedicated frequencies of the VM. It is demonstrated that in the region, where the *H–O* bond breaking always takes place, there exist the *H–H* bond stability islands. Optimum parameters of VM dissociation have been determined.

**KEY WORDS:** virtual water molecule, eigenfrequencies, bond length, atomic mass, external force, dissociation.

## ДИССОЦИАЦИЯ ВИРТУАЛЬНОЙ МОЛЕКУЛЫ ВОДЫ ВО ВНЕШНИХ ЭЛЕКТРОМАГНИТНЫХ ПОЛЯХ

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В работе предложена модель описания реальной молекулы воды ее двумерным аналогом – виртуальной молекулой (ВМ). В предложенной модели ВМ обеспечено условие совпадения основных собственных частот молекулы и ее аналога. Остальные параметры ВМ (длина связей и массы атомов) перенормированы таким образом, чтобы молекула устойчиво существовала длительный интервал времени. Исследована линейная динамика атомов ВМ в поле монохроматической электромагнитной волны. Показано, что при воздействии внешнего электромагнитного поля на молекулу на резонансной частоте наблюдаются секулярные режимы колебаний, которые характеризуются линейным во времени ростом амплитуд колебаний атомов. Исследовано влияние включения внешней силы в момент установления собственных колебаний ВМ на устойчивость колебаний ее атомов. Показано, что в некоторых случаях разрыв одной из связей ВМ неизбежно приводит к ее распаду в целом. В результате численного моделирования установлено, что разрыв связей имеет пороговый характер, т.е. диссоциация не наблюдается при внешней силе, меньшей определенного значения. В области сил, превышающих пороговые, варьирование частоты внешнего электромагнитного поля не чувствительно к резонансным эффектам, обусловленным наличием выделенных частот у ВМ. Показано, что в области, где всегда происходит разрыв связи *H–O* существуют островки стабильности связи *H–H*. Определены оптимальные параметры диссоциации ВМ.

**КЛЮЧЕВЫЕ СЛОВА:** виртуальная молекула воды, собственные частоты, длина связи, атомная масса, внешняя сила, диссоциация

## ДИСОЦІАЦІЯ ВІРТУАЛЬНОЇ МОЛЕКУЛИ ВОДИ В ЗОВНІШНІХ ЕЛЕКТРОМАГНІТНИХ ПОЛЯХ

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У роботі запропонована модель опису реальної молекули води її двовимірним аналогом - віртуальною молекулою (ВМ). У запропонованій моделі ВМ забезпечена умова збігу основних власних частот молекули і її аналога. Інші параметри ВМ (довжина зв'язків і маси атомів) перенормовані таким чином, щоб молекула стійко існувала тривалий інтервал часу. Досліджено лінійну динаміку атомів ВМ у полімонохроматичної електромагнітної хвилі. Показано, що при впливі зовнішнього електромагнітного поля на молекулу на резонансній частоті спостерігаються секулярні режими коливань, які характеризуються лінійним у часі зростанням амплітуд коливань атомів. Досліджено вплив включення зовнішньої сили в момент установлення власних коливань ВМ на стійкість коливань її атомів. Показано, що в деяких випадках розрив однієї з

зв'язків VM неминуче приводить до її розпаду в цілому. У результаті числового моделювання встановлено, що розрив зв'язків має граничний характер, тобто дисоціація не спостерігається при зовнішній силі, меншій певного значення. В області сил, що перевищують граничні, варіювання частоти зовнішнього електромагнітного поля не відчутно до резонансних ефектів, обумовлених наявністю виділених частот у VM. Показано, що в області, де завжди відбувається розрив зв'язку  $H-O$ , існують острівці стабільності зв'язку  $H-H$ . Визначено оптимальні параметри дисоціації VM.

**КЛЮЧОВІ СЛОВА:** віртуальна молекула води, власні частоти, довжина зв'язку, атомна маса, зовнішня сила, дисоціація

Today, many economically advanced countries are more closely consider hydrogen not only in the traditional application, but also as a basis for energy tomorrow. Against the background of the catastrophic environmental degradation and depletion of the world hydrocarbon resources, it is tempting to use hydrogen as a fuel is harmless to the means of transport, heating in remote regions, autonomous and stationary sources of secondary energy. Hydrogen is chosen as the most abundant element on the earth and in space, but in nature it almost does not occur in pure form and must be extracted from chemical compounds ( $H_2O$ ,  $HCl$ ,  $HF$ , etc.)

Triatomic molecules ( $H_2O$ ,  $CO_2$ ,  $NO_2$ ,  $SO_2$ ,  $H_2S$ , etc.) are characterized by the presence of a fine structure of their absorption spectra. A full and exact information on the parameters of these spectra is of basic importance for solving many applied and fundamental problems such as the development of theory and practice of femtochemistry [1]; analysis of the impact of volcanic outbursts, “greenhouse” effect, ozone layer on the ecology and climate variations of the Earth [2]; creation of alternative energy sources based on the controlled molecule dissociation in external electromagnetic fields [3,4].

One of the methods to control the internal dynamics of triatomic molecules is to act upon them through an electromagnetic field, which is oscillating at frequencies close to the frequencies of atomic oscillations in molecules [3,4]. Since the frequencies of atomic oscillations in molecules lie in the infrared spectrum [5], the resonance action on the internal dynamics of the molecule is entirely feasible with the use of lasers that generate electromagnetic radiation of corresponding wave lengths [1].

The other method of water molecule dissociation, different from laser technologies, has been described by Meyerin his patent [6]. Here, to achieve the objective, a sequence of special-shape unipolar voltage pulses was used, with the voltage-time step function for the leading and trailing edges of the pulse and the exponentially increasing function for the pulse peak.

Since the above-described methods of triatomic molecule dissociation by external electromagnetic fields are far from creating of adequate model [3,4] or are based on empirical facts [6], it appears of importance and necessity to continue the research in this direction. The present paper deals with the modeling of the interaction between the real triatomic molecule ( $H_2O$  as an example) and the external electromagnetic fields of the virtual molecule (VM).

The aim of this work is a study of the steady state of virtual water molecules, which simulates a real molecule of water, and determination of its dissociation conditions in external electromagnetic fields.

### THE MODEL OF WATER MOLECULE

The water molecule presents a triatomic molecule  $H_2O$  that consists of one oxygen atom and two hydrogen atoms. Its schematic view is shown in Fig. 1.

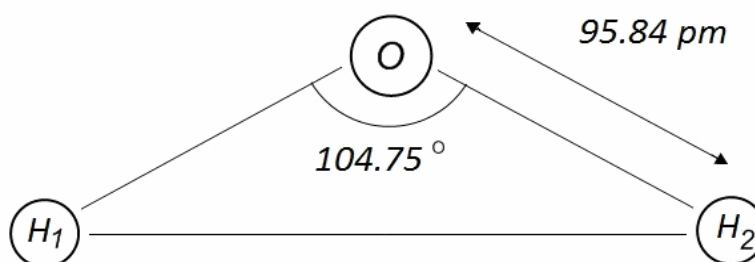


Fig. 1. Scheme of water molecule

The oxygen atoms are linked with the hydrogen atom by covalent chemical bonds, each bond involving two electrons (in the figure, the bonds are shown by lines). The equilibrium length of the  $H-O$  bond makes 0.9584 Å. The valence angle (angle between valence bonds) is equal to  $104.75^\circ$  [4]. The  $H-O$  bond energy is determined to be 101.3 kcal/mole [7]. This energy is also called the dissociation energy, because its excess leads to bond breaking, and that corresponds to the molecule dissociation.

### DETERMINATION OF FICTITIOUS $H-H$ BOND COEFFICIENT AND VM PARAMETERS

Similarly to ref. [8], we consider a planar (two-dimensional) model of water molecule. We shall represent the atoms by point masses, denoting the hydrogen atomic mass by  $m_H$ , and the oxygen atomic mass by  $m_O$ . In the equilibrium state, the hydrogen atoms are situated at the ends of the base of the isosceles triangle, and the oxygen atom is found at the vertex of the angle formed by its lateral sides. We introduce the notation  $a_{HO}$  and  $a_{HH}$ , which correspond

to the equilibrium distance between the oxygen atom and the hydrogen atom, and between hydrogen atoms, respectively.

In the centre-of-mass system (C.M.S.) the equations of motion for the molecule atoms being in the external electromagnetic field are written as

$$\begin{cases} m_H \frac{d^2 \vec{R}_{H_1}}{dt^2} = \vec{F}_{H_1} + \vec{F}_{H_1O} + \vec{F}_{H_1H_2}, \\ m_O \frac{d^2 \vec{R}_O}{dt^2} = \vec{F}_O + \vec{F}_{OH_1} + \vec{F}_{OH_2}, \\ m_H \frac{d^2 \vec{R}_{H_2}}{dt^2} = \vec{F}_{H_2} + \vec{F}_{H_2O} + \vec{F}_{H_2H_1}. \end{cases} \quad (1)$$

Here  $\vec{R}_O = \{X_O, Y_O\}$ ,  $\vec{R}_{H_1} = \{X_{H_1}, Y_{H_1}\}$  и  $\vec{R}_{H_2} = \{X_{H_2}, Y_{H_2}\}$  are the radii-vectors of oxygen and hydrogen atoms, drawn from the centre of mass;  $\vec{F}_O, \vec{F}_{H_1}, \vec{F}_{H_2}$  are the vectorial forces of electromagnetic field action on oxygen atoms;  $\vec{F}_{H_1O}, \vec{F}_{OH_1}, \vec{F}_{H_2O}, \vec{F}_{OH_2}, \vec{F}_{H_1H_2}, \vec{F}_{H_2H_1}$  are the vectorial action forces of atoms indicated by the first on the atoms indicated by the second.

We suppose that the electromagnetic field can be described by a monochromatic wave propagating in the assigned direction, and take into consideration only the electric field strength. Since the treatment is carried out in the C.M.S., and the molecule is immobile, then the total action of the electric field strength on the molecule equals zero. In this case, the following equalities may be considered as fulfilled for the moduli of external forces:

$$|\vec{F}_{H_1}| = |\vec{F}_{H_2}| = -\frac{1}{2} |\vec{F}_O| \equiv |F|. \quad (2)$$

The external force direction  $\vec{F}$  is given by the unit vector  $\vec{e}$ :  $\vec{F} = |\vec{F}| \cdot \vec{e}$ , and the force value is given by the relation:  $|\vec{F}| \approx d' \cdot E(t)$ , where  $d'$  - is the derivative of the dipole  $H-O$  bond moment with respect to the interatomic distance, is the electric field strength amplitude prescribed externally.

For intramolecular forces the relationship  $\vec{F}_{AB} = -\vec{F}_{BA}$  is valid.

We now determine the intramolecular force values proceeding from the assumption that the forces are paired and central. The assumption is corresponds to the Morse potential representation of the interaction force field [8]

$$\Pi_{AB}(\vec{r}) = D_{AB} (\exp(-2\alpha_{AB}(r - a_{AB})) - 2 \exp(\alpha_{AB}(r - a_{AB}))), \quad (3)$$

where  $D_{AB} = D_{BA}$  is the binding energy between the atoms  $A$  and  $B$ ,  $\alpha_{AB} = \alpha_{BA}$  is the equilibrium distance between them,  $a_{AB} = a_{BA}$  is the parameter describing the width of potential well.

Using eq. (3) we can determine the value and direction of force between the atoms  $A$  and  $B$ :

$$\vec{F}_{AB} = -\frac{d}{dr} \Pi_{AB}(\vec{R}_A - \vec{R}_B) \frac{\vec{R}_A - \vec{R}_B}{|\vec{R}_A - \vec{R}_B|}. \quad (4)$$

The analysis of a linearized set of equations (1) in the absence of the external electromagnetic field and with due regard for eq. (4) leads to the following equations for the eigenfrequencies:

$$(2m_O \alpha_{HO}^2 + m_O \alpha_{HH}^2) C_{HO} - 2m_H m_O \alpha_{HO}^2 \omega^2 = 0 \quad (5)$$

$$2\alpha_{HO}^2 m_O m_H^2 \omega^4 + (m_H^2 \alpha_{HH}^2 C_{HO} - 4m_H^2 \alpha_{HO}^2 C_{HO} - 4m_O m_H \alpha_{HO}^2 C_{HH} - 2m_O m_H \alpha_{HO}^2 C_{HO}) \omega^2 + 4m_O \alpha_{HO}^2 C_{HO} C_{HH} + 8m_H \alpha_{HO}^2 C_{HO} C_{HH} - m_O \alpha_{HH}^2 C_{HO} C_{HH} - 2m_H \alpha_{HH}^2 C_{HO} C_{HH} = 0, \quad (6)$$

where  $C_{AB} = 2\alpha_{AB}^2 D_{AB}$  are the stiffness factors of molecule bonds.

If in Eqs. (5,6) all the parameters were prescribed, then it would be possible to determine from them the eigenfrequencies of antisymmetric  $\omega_{as}$  (eq. (5)) and symmetric  $\omega_s^{(1)}$ ,  $\omega_s^{(2)}$  (Eq. (6)) molecular oscillations.

However, in our case we have only the experimentally measured eigenfrequencies, molecular dimensions  $\alpha_{OH}$ ,  $\alpha_{HH}$  and the bond energy  $D_{OH}$ . Their values are listed in Table 1 [9, 10].

The Tabl. 2 gives the width values of potential wells  $\alpha_{AB} \equiv \sqrt{C_{AB}(2D_{AB})^{-1}}$  in the Morse representation. Note that

to calculate the unknown width of the  $H-H$  bond potential well, we assume the relation  $D_{HH} \approx 0,2 \cdot D_{HO}$  to be true [4].

Table 1.

Equilibrium parameters of the nitrogen dioxide molecule

Parameter	Notation	Values	
		SI units	Hartree units
Oxygen atomic mass	$m_O$	$2.657 \cdot 10^{-26}$ kg	29176
Hydrogen atomic mass	$m_H$	$1.6737 \cdot 10^{-26}$ kg	18373
H – O bond dissociation energy	$D_{HO}$	101.3 kcal/mole	0.1614
H – O bond equilibrium distance	$\alpha_{OH}$	0.93 Å	1.81474
H – H bond equilibrium distance	$\alpha_{HH}$	1.53 Å	2.8922
Antisymmetric vibration frequency	$\omega_0 \equiv \omega_a$	$3938.7 \text{ cm}^{-1}$	$17.92 \cdot 10^{-3}$
Symmetric vibration frequency	$\omega_1 \equiv \omega_s^{(1)}$	$3835.4 \text{ cm}^{-1}$	$17.45 \cdot 10^{-3}$
	$\omega_2 \equiv \omega_s^{(2)}$	$1647.6 \text{ cm}^{-1}$	$7.49 \cdot 10^{-3}$

Since the eigenfrequencies have been observed and measured for the real molecule, for the transition from its three-dimensional model to the planar one some parameters must be renormalized, i.e., they should be changed so that eqs. (5), (6) should become jointly. As a result of these manipulations, the parameters of the two-dimensional VM would be determined, with the use of which the processes in the real molecule could be modeled.

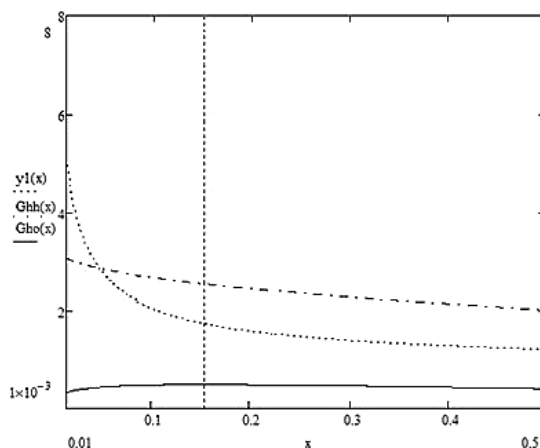


Fig. 2. Solution of eq. (9) for  $y$  versus  $x$ , and the molecule stiffness factor  $G_{ho} \cdot 10^5$  and  $G_{hh} \cdot 10^5$  as a function of the parameter  $x$ .

For this purpose we assume the eigenfrequencies  $\omega_i$  in eqs. (5), (6) be prescribed, and the parameters that have to

be determined (i.e., their new values should be found (renormalized)), will be put to be  $x = \frac{m_H}{m_O}$ ;  $y = \frac{1}{2} \left( \frac{\alpha_{HH}}{\alpha_{OH}} \right)^2$ . In

this case, the stiffness factors  $C_{HH} \cdot m_H^{-1}$  and  $C_{HO} \cdot m_H^{-1}$  are expressed in terms of the eigenfrequencies  $x, y$  in the following way:

$$G_{HO} = C_{HO} \cdot m_H^{-1} = \frac{\omega_0^2}{1 + xy} \quad (7)$$

$$G_{HH} = C_{HH} \cdot m_H^{-1} = \frac{1}{2} (\omega_0^2 + \omega_1^2 + \omega_2^2) - \frac{1+x}{1+xy} \omega_0^2. \quad (8)$$

Transforming eq. (6) with regard for eqs. (7), (8) it is not difficult to derive the required equation, which relates the renormalized parameters  $x, y$  (Fig. 2.):

$$Z^2(x, y) - Z(x, y)(1+x)(1+y) + 1 + x(2-y) - \left( \frac{1+xy}{2} \right)^2 \left( \left( \frac{\omega_1}{\omega_0} \right)^2 - \left( \frac{\omega_2}{\omega_0} \right)^2 \right)^2 = 0, \quad (9)$$

where

$$Z(x, y) = \frac{1+xy}{2} \left( 1 + \left( \frac{\omega_1}{\omega_0} \right)^2 + \left( \frac{\omega_2}{\omega_0} \right)^2 \right) - x - 1.$$

As in [8] were calculated parameters of virtual molecules listed in Table 2.

Table 2.

VM parameters

Parameter	Notation	Hartree units
Oxygen atomic mass (renormalized)	$m_O^*$	149967
Hydrogen atomic mass	$m_H$	18373
$O-H$ bond stiffness factor	$C_{OH}$	4.658
$H-H$ bond stiffness factor	$C_{HH}$	0.885
Equilibrium length of the $O-H$ bond (renormalized)	$\alpha_{OH}^*$	1.557
Equilibrium length of the $H-H$ bond	$\alpha_{HH}$	2.8922
Width of potential well for the $H-O$ bond	$\alpha_{HO}$	3.798
Width of potential well for the $H-H$ bond	$\alpha_{HH}$	3.703

### LINEAR DYNAMICS OF VM ATOMS IN THE FIELD OF MONOCHROMATIC ELECTROMAGNETIC WAVE

We write down the external force created by the electromagnetic wave field, which exerts action on the molecule atoms, as:

$$|\vec{F}| = d' \cdot E(t) \cdot \vec{e} \equiv d' \cdot E_0 e^{-i(\omega t + \theta)} \cdot \vec{e}, \quad (10)$$

where  $E_0, \omega, \theta$  are, respectively, the amplitude, frequency and control phase of the electric field strength of the wave.

Let us investigate the linear response of the molecule to the action of the external electromagnetic field. To this end, we derive the equation describing the temporal variation of the bond lengthening  $X_{H_1O} \equiv \delta \vec{R}_{H_1} \cdot \vec{e}_{H_1O}$ , which characterizes small deviations of the hydrogen atom  $H_1$  from the equilibrium position along the  $O-H_1$  bond. In this case it is necessary to use the VM parameters presented in Table 2.

Since in the proposed model the atoms of water molecule are described by the triangle with the corresponding stiffness coefficients, to estimate the dynamic strength of this structure, it will suffice to have information about the lengthening of one of the bonds, e.g.,  $O-H_1$ .

After linearization of the initial set of equations (1), assuming the peak value of force  $|\vec{F}_d| \equiv d' \cdot E_0(t)$  to be the function weakly dependent on time ( $\frac{dE_0}{dt} \ll \omega E_0$ ), we obtain the equation that describes the temporal variation of the bond lengthening  $X_{H_1O}$  under the action of the external field with the frequency  $\omega_0$ :

$$\frac{d}{dt} X_{H_1O} = -\frac{F_d}{2} \frac{C_{HO}(1 + 2\frac{m_H}{m_O^*})}{m_H^2 \omega_H^3} \cos \phi_0 \cos \varphi, \quad (11)$$

where  $\phi_0 \approx 37.625^\circ$  is the renormalized angle at the base of the molecule,  $\varphi$  is the angle between the external force direction and the  $H_1-H_2$  direction, is the time in Hartree units,  $\theta = -\frac{\pi}{2}$ .

It is not hard to show that the lengthening of oxygen bonds with other atoms of the molecule is determined through  $X_{H_1O}$  in the following way:

$$\delta \vec{R}_{H_1} \cdot \vec{e}_{H_2O} \gamma^{-1} = \delta \vec{R}_{H_1} \cdot \vec{e}_{H_1H_2} \beta^{-1} = -\delta \vec{R}_{H_2} \cdot \vec{e}_{H_1O} \gamma^{-1} = -\delta \vec{R}_{H_2} \cdot \vec{e}_{H_2O} = \delta \vec{R}_{H_2} \cdot \vec{e}_{H_1H_2} \beta^{-1} = \delta \vec{R}_{H_1} \cdot \vec{e}_{H_1O}, \quad (12)$$

where  $\beta = \frac{a_{HH}}{2a_{OH}^*} = 0.929$ ,  $\gamma = \left( \frac{a_{HH}}{a_{OH}^*} \right)^2 = -0.726$ .

From eq. (11) it follows that the  $O-H_1$  bond length increases linearly with time at the angles of action  $\frac{\pi}{2} < \varphi < \frac{3\pi}{2}$ . The length of other bonds also changes with time by the linear law in accord with relations.

Thus, the presence of secular regimes in eq. (11), which result from the action of the external electromagnetic field on the molecule at a resonance frequency, points to the adequacy of the proposed model to the physical processes, which are to take place in the real molecule.

Since the linear dynamics of the molecule displays its resonant properties, it appears of interest to retrace the VM behavior at great atomic displacement amplitudes, i.e., to investigate VM nonlinear oscillations up to the bond breaking.

### NONLINEAR DYNAMICS AND DISSOCIATIVE MODES OF THE VM IN THE MONOCHROMATIC ELECTROMAGNETIC WAVE FIELD

#### Nonlinear dynamics of the VM

The investigation on the VM nonlinear dynamics in external fields must be started from the adjustment of nonlinear oscillations of a free molecule, i.e., from initial data fitting in the original equations (1) in the absence of external fields. As a result of this adjustment, the VM oscillation spectrum must comprise eigenfrequencies  $\omega_i$ . In this case, the initial arrangement of VM atoms must be in accord with the linear theory.

The numerical calculation data on the temporal change of VM atom coordinates as well as their spectral resolution are presented in Fig. 3,4. It follows from these figures that with time the molecular atoms fit into the parameters of the Morse potential, i.e., oxygen atoms oscillate relative to the points with the coordinates  $X_O \approx 0.0$ ;  $Y_O \approx 0.057$  and the hydrogen atom oscillates relative to the point with the coordinates  $X_{H1,H2} \approx \pm 1.44735$ ;  $Y_{H1,H2} \approx -0.4917$ .

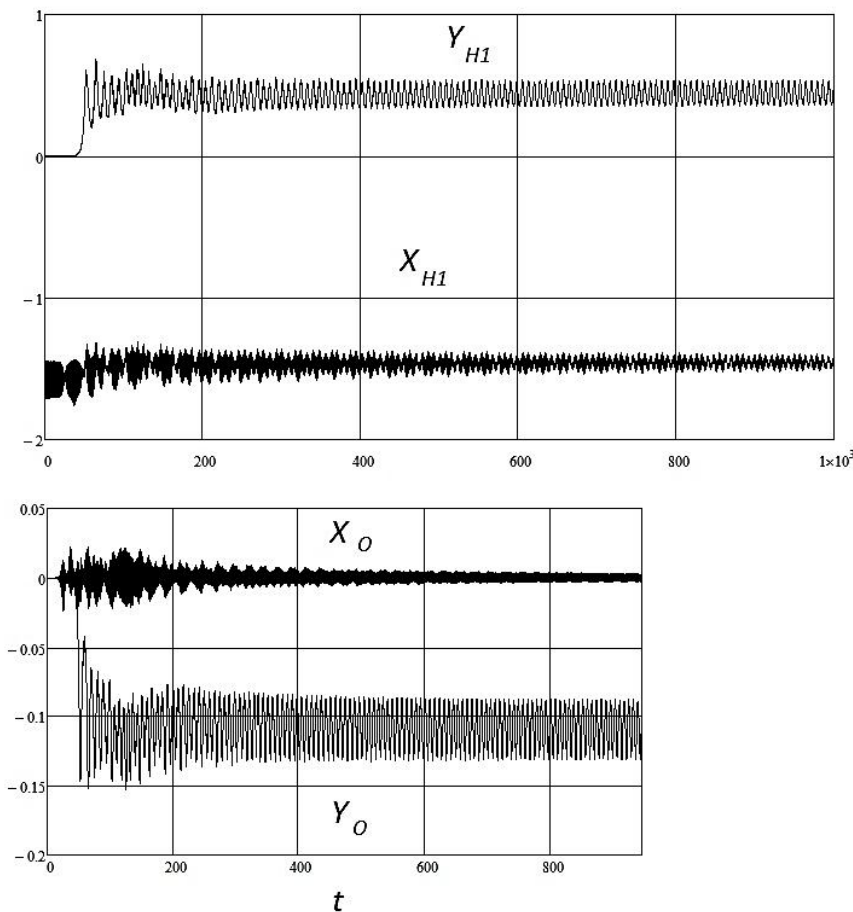


Fig. 3. Coordinates of hydrogen and oxygen atoms in the molecule versus time  $t$ .

The VM oscillation spectrum intensity  $I_\Omega$  was obtained by the use of a fast Fourier transform of atomic displacement projections in the  $x, y$ , coordinates, calculation of their arithmetic mean and a subsequent moving average smoothing (Fig. 4). For identification of peaks of the thus obtained spectrum we make use of the fact that the maximum resonance frequency  $\Omega_0$  should have the peak intensity (Very Strong), and the lowest frequency  $\Omega_2$  should have a lower intensity (Strong).

In view of the above, the spectrum analysis permits us to separate the following resonance frequencies of VM oscillations:  $\Omega_0 \approx 0.13916$ ;  $\Omega_1 \approx 0.27588$ ;  $\Omega_2 \approx 0.41016$  which the appropriate choice of a new mass of an oxygen atom  $m'_0$  equivalent to the eigenfrequencies  $\omega_2$ . So, the data given in Fig. 4, show that the proposed model adequately describes nonlinear nitrogen dioxide molecular oscillations: the eigenfrequencies of VM oscillations correspond to the frequencies of symmetrical and antisymmetrical oscillations of real nitrogen dioxide.

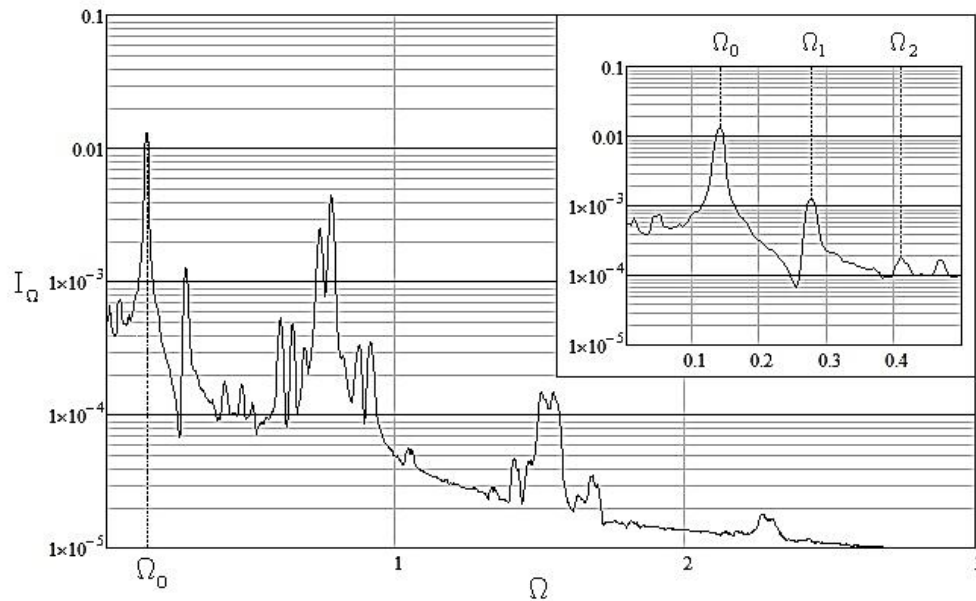


Fig. 4. Averaged and smoothed intensities  $I_{\Omega}$  of the oscillation spectrum of water VM atoms. After appropriate transformations, the peaks, marked with dashed lines, coincide with resonant frequencies of the real water molecule  $\omega_i$ .

#### VM dissociative modes in the field of a monochromatic electromagnetic wave

Examine dissociative modes VM fields of external electromagnetic radiation. To do this, at the moment the eigenfrequencies of the VM to include the external force. The force value is determined by expression (10), where the control phase may equal zero, and the force direction is prescribed by the unit vector  $\vec{e}$ .

As it follows from the calculations, at the moment of external force switch on, the molecule atoms oscillate in the neighborhood of vertices of the isosceles triangle with the coordinates  $X_{H1,H2} \approx \pm 1.44735$ ;  $Y_{H1,H2} \approx -0.4917$ ;  $X_O \approx 0.0$ ;  $Y_O \approx 0.057$ . This state of the VM will be characterized as equilibrium.

In numerical calculations, the harmonic component of the external force is prescribed in the form of  $\approx F \cdot \sin(\Omega t)$ , where the amplitude  $F$  varies in the range  $0 \leq F \leq 3$ , and the angle of force action  $\varphi$  ranges within  $0 < \varphi < 2\pi$ .

In calculations, we shall assume that an increase in the  $H-H$  or  $H-O$  bond length by more than two times leads to bond breaking. And if one takes into account that all the calculations are carried out in the C.M.S., then the breaking of one of the bonds gives such a reactive force to the other VM atoms, that it inevitably results in the VM dissociation as a whole. This conclusion is confirmed by numerical simulation, too.

The main question of numerical simulation of VM dynamics in the field of external forces consists only in what bond will be the first to break and at what conditions. The answer to this question is given by numerical simulation of atom dynamics of the triatomic VM in the field of the external electromagnetic wave.

Fig. 5-8 show the numerical simulation results for VM bond dissociation versus the  $F$  amplitude and the angle of action of the external force,  $\varphi$  specified by both the electromagnetic wave (Fig. 5-7) and the stationary electric field (Fig. 8). In the figures, the bottom plane specifies the parameters of the  $H-H$ , bond breaking, and the top plane –  $H-O$  bond breaking. The areas in the planes, marked by small squares with a side length of 0.1, correspond to these bond breakings.

The data presented in Fig. 5-8 are characterized by the periodicity in the angle of external force action  $\varphi$ .

From Fig. 5-7 it follows that for all resonance frequencies the bond dissociation does not take place at the external force lower than a certain value  $F \leq 0.5 \div 0.8$ , the range of this value being dependent on the angle  $\varphi$ .

At  $F \geq 0.8$  the change in the frequency of the external electromagnetic field gives no resonance effects specified by the presence of dedicated frequencies of the molecule.

This may be due to a strong nonlinear link of atoms in the molecule, when linear connections cannot manifest themselves. The observed correlation of minimum forces  $F$ , leading to breaking of  $H-H$  and  $H-O$  bonds, can also be attributed to a strong nonlinear link of atoms in the molecule.

From Fig. 5-7 it can be seen that at  $F > 0.4$  the  $H-O$  bond breaking always takes place, whereas the  $H-H$  bond may exhibit the stability islands. This is particularly evident for the resonance frequency  $\Omega_0$ , which is characterized by the maximum amplitude of oscillations.

Since the VM dissociation occurs at breaking of any bond, it is of interest to find the optimum parameters of dissociation, viz., the minimum force and the corresponding to it angle of action on the molecule.

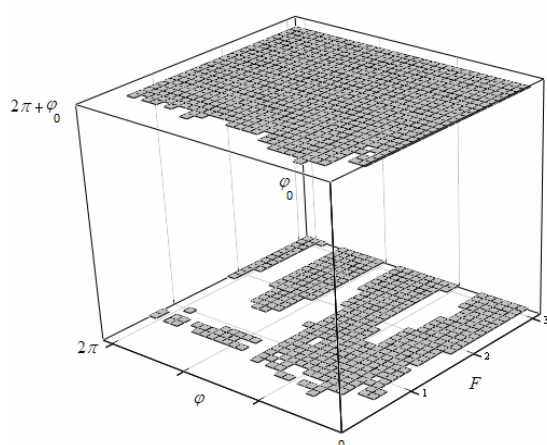
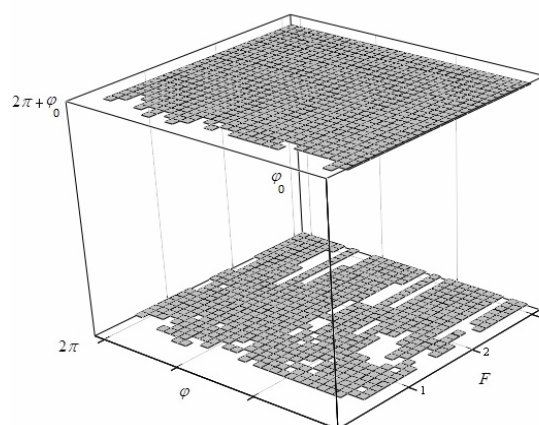
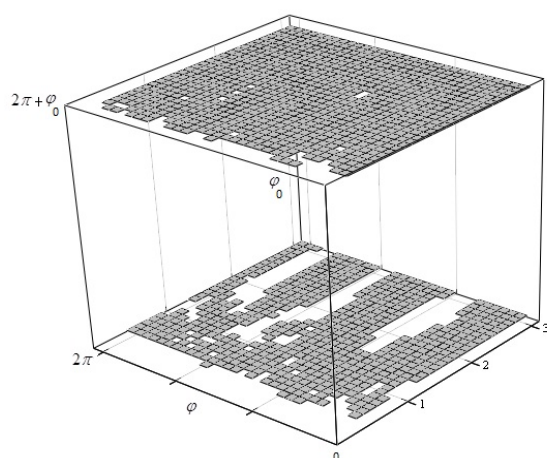
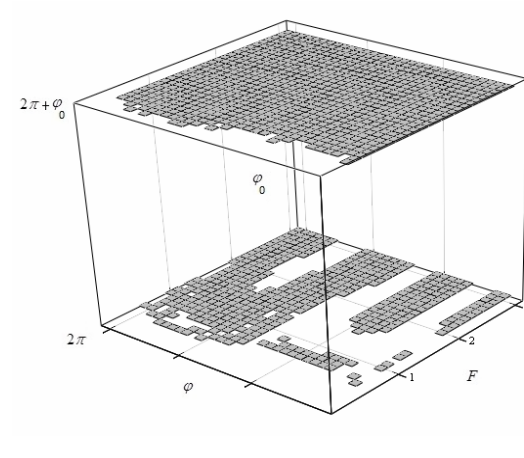
Fig. 5. Electromagnetic field frequency  $\Omega_0$ .Fig. 6. Electromagnetic field frequency  $\Omega_1$ .Fig. 7. Electromagnetic field frequency  $\Omega_2$ .

Fig. 8. The electromagnetic field is constant.

The numerical simulation data on the optimum parameters of dissociation are presented in Table 3.

Table 3.

Optimum VM dissociation parameters

Electromagnetic wave field of the frequency, $\Omega$	Force, $F$	Angle of action, $\varphi$
$\Omega_0$	0.4	$\pi(4/15) \leq \varphi \leq \pi(2/5)$
$\Omega_1$	0.4	$\pi(23/15) \leq \varphi \leq \pi(49/30)$
$\Omega_2$	0.4	$\pi(16/15) \leq \varphi \leq \pi(61/30)$ $\pi(26/15) \leq \varphi \leq \pi(61/30)$
Constant field	0.3	$\pi(46/30) \leq \varphi \leq \pi(49/30)$

Theoretical studies have shown that the development of the experimental cell needs to apply a constant field with a rectangular pulse of force  $F = 0.3$  in units of Hartree in the Si units  $F = 2.2$  V/cm and at angles of impact of  $\pi(46/30) \leq \varphi \leq \pi(49/30)$ .

### CONCLUSIONS

Thus, we have proposed the model for description of the real water molecule by its two-dimensional analog, namely, the virtual molecule (VM). In the proposed VM model, the condition of coincidence between the eigenfrequencies of the molecule and its analog is provided. The other VM parameters (bond length and atomic mass) are renormalized so that the molecule should steadily exist for a long time interval.

Linear dynamics of VM atoms in the field of a monochromatic electromagnetic wave has been investigated. It has been shown that under the action of an external electromagnetic field on the molecule at a resonance frequency, secular regimes of oscillations are observed. The last ones are characterized by a time-linear growth of atomic oscillation amplitudes. The increase in the atomic oscillation amplitudes places the molecule in the nonlinear regime. Under these



conditions, the dynamics of VM atoms in the field of the monochromatic electromagnetic wave causing the VM dissociation can be investigated only by the numerical simulation method. To this end, after the VM eigenfrequencies settled, the action of the external force on the molecule dissociation was investigated. It has been demonstrated that in some cases the breaking of one of VM bonds inevitably leads to the VM dissociation as a whole. As a result of numerical simulation, it has been established that the bond breaking has a threshold character, i.e., dissociation is not observed at the external force, which is lower than a certain value of  $F \leq 0.3 \div 0.7$ . The range of external force variations depends on the angle of external action  $\varphi$ . In the range of forces exceeding the threshold values,  $F > 0.7$  the variation in the external electromagnetic field frequency is insensitive to the resonance effects that are due to the presence of dedicated frequencies of the VM. It has been demonstrated that at  $F > 0.4$  the  $H-O$  bond breaking always takes place, whereas the  $H-H$  bond may exhibit stability islands. Optimum parameters of VM dissociation have been determined and set parameters of the experimental cell.

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