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NEW QUANTUM APPROACH TO DETERMINATION OF THE MOLECULAR SPECTRAL CONSTANTS AND PROBABILITIES FOR COOPERATIVE VIBRATION-ROTATION-NUCLEAR TRANSITIONS IN SPECTRA OF DIATOMICS AND THE HADRONIC MOLECULES

It is proposed a new approach to construction of the potential function of diatomic molecules as a sum of the known perturbed Morse oscillator function, the Simons-Parr-Finlan molecular potential in the middle of the potential curve, function of the $-C_n/R^n$ type at the large internuclear distances. Within this approach it is presented a precise scheme for computing the molecular spectral parameters, namely, vibrational, rotational, centrifugal constants for the electronic states of diatomics. As application it was carried out calculation of the of molecular constants (cm-1) for the $X^1\Sigma^+$ $B^1\Pi$ states of the KRb dimer and rubidium dimer and performed further comparison with experimental data. Within consistent approach to calculation of the electron-nuclear γ transition spectra (set of vibration-rotational satellites in molecule) of molecule there are obtained the estimates for vibration-rotation-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{127}I ($E^{(0)\gamma}= 203$ keV) in the molecule of $H^{127}I$ for different approximations of the for potential curves: the harmonic oscillator, the Dunham model and presented approach.

From physical viewpint it is obvious that any alteration of the molecular state must be manifested in the quantum transitions, for example, in a spectrum of the *g*-radiation of a nucleus (see for example [1-9]). In result of the gamma nuclear transition in a nucleus of a molecule there is arised a set of the electron-vibration-rotation satellites, which are due to an alteration of the state of the molecular system interacting with photon. The known example is the Szilard-Chalmers effect which results to molecular dissociation because of the recoil during radiating gamma quantum with large energy.

In series of works [3-9] it has been carried out detailed studying the co-operative dynamical phenomena due the interaction between atoms, ions, molecule electron shells and nuclei nucleons. There have been developed a few advanced approaches to description of a new class of dynamical laser-electron-nuclear effects in molecular spectroscopy, in particular, a nuclear gamma-emission or absorption spectrum of a molecule. A consistent quantum- mechanical approach to calculation of the electron-nuclear g transition spectra (set of vibration-rotational satellites in molecule) of a nucleus in the multiatomic molecules has been earlier proposed [5,7] and generalizes the well known approach by Letokhov-Minogin [4]. Earlier there were have been obtained estimates and calculations of the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{191}Ir ($E^{(0)}_g = 82$ keV) in the molecule of IrO_4, ^{188}Os ($E^{(0)}_g = 155$ keV in OsO_4 and other molecules were listed. In Ref [8] there are firstly presented theoretical data on the vibration-nuclear transition

probabilities in a case of the emission and absorption spectrum of the nucleus of rhenium ^{186}Re ($E^{(0)}_g$ = 186.7 keV) in the molecule of ReO_4, estimated on the basis of the simplified version [5,7] of the consistent quantum-mechanical approach to co-operative electron-g-nuclear spectra (a set of the vibration-rotational satellites in a spectrum of molecule) of multiatomic molecules.

In this paper we present a genetralization of the cited theory of cooparative electron-gamma-nuclear (vibrational, rotational) transitions in a case of the diatomic moleules using new principle of construction of the potential curves for diatomic, which is in some degree analogous to the Smirnov approach [10,11]. Moreover the proposed method allow to determine the molecular spectral parameters, that ic checked on the example of the some alkali dimers. Besides, we will give a short generalization of the theory on a case of the exotic hadronic (pionic) molecules.

It should be noted that the diatomics potential function can be obtained on the decision of the electronic Schrödinger equation, however, due to significant computational difficulties in the present, this problem is reliably solving only for the case of the simplest diatomics having a small number of electrons [10-15]. In this regard, the first promising more used semi-empirical methodsy, where the potential curves are determined in the adiabatic approach using experimental vibrational and rotational spectroscopic constants. Some authors have studied solutions of the Schrodinger (or Klein-Gordon) equation with some known physical potential models, such as the Morse potential, Rosen-Morse potential, Manning-Rosen potential, Poschl-Teller potential, Deng-Fan potential, ring-shaped potential, and hyperbolic Scarf potential etc (look details for example in Ref. [10,16-18]).

Ler us remind shortly a scheme for computing the cooperative on the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of the nucleus of diatomics as the corresponding method is earlier presented in details (look [5-8]). The aim is to compute parameters of the gamma transitions (a probability of transition) or spectrum of the gamma satellites because of changing the electron-vibration-rota-tional states of the molecule under gamma quantum radiation (absorption).

Our purpose is calculation of a structure of the gamma transitions (probability of transition) or spectrum of the gamma satellites because of the changing the electron-vibration-rotational states of diatomic molecules under the gamma quantum radiation (absorption). In adiabatic approximation a wave function of molecule is multiplying the electronic wave function and wave function of nuclei: $y(r_e)y(R_1,R_2)$. Hamiltonian of interaction of the gamma radiation with system of nucleons for the first nucleus can be expressed through the co-ordinates of nucleons r_n' in a system of the mass centre of the first nucleus [4,7]:

$$H(r_n) = H(r_n{}') \exp(-ik_\gamma R_1) \qquad (1)$$

where k_g is a wave vector of the gamma quantum. The matrix element for transition from initial state "a" to final state "b" is presented as usually:

$$< \Psi^*_b(r_n) | H(r_n) | \Psi_a(r_n) > \bullet$$

$$\bullet < \Psi^*_b(r_e) \Psi^*_b(R_1,R_2) | e^{-ik_\gamma R_1} | \Psi_a(r_e) \Psi_a(R_1,R_2) > \quad (2)$$

The first multiplier in (1) is defined by the gamma transition of nucleus and is not dependent upon an internal structure of molecule in a good approximation. The second multiplier is a matrix element of transition of the molecule from initial state "a" to final state "b":

$$M_{ba} = < \Psi^*_b(r_e) | \Psi_a(r_e) > \bullet$$
$$\bullet < \Psi^*_b(R_1,R_2) | e^{-ik_\gamma R_1} | \Psi_a(R_1,R_2) > \qquad (3)$$

The expression (7) gives a general formula for calculation of the probability of changing internal state of molecule under absorption or emitting gamma quantum by nucleus of the molecule and defines an amplitude of the corresponding gamma satellites. Their positions are fully determined by the energy and pulse conserving laws as follows [2]:

$$\pm E_\gamma + E_a + (1/2)Mv_0^2 = \pm E_\gamma^{(0)} + E_b + (1/2)Mv^2 \quad (4)$$
$$Mv_0 \pm \hbar k_\gamma = Mv$$

Here M is the molecule mass, v_0 and v are velocities of molecule before and after interaction of

nucleus with g quantum, E_a and E_b are the energies of molecule before and after interaction, E_g is an energy of nuclear transition. Then an energy of the g satellite is as follows):

$$E_\gamma = E_\gamma^{(0)} + \hbar k_\gamma v_0 \pm R_{om} \pm (E_b - E_a) \quad (5)$$

Here R_{om} is an energy of recoil: $R_{om} = [(E_g^{(o)}]^2/2Mc^2$. It is well known (c.f.[4,7]) that the practical interest are presented only transitions between vibration-rotational levels of the ground electron state, including transitions into continuum with further molecular dissociation. The matrix element of transition for these transitions is

$$M_{ba} = <\Psi_b^*(R_1, R_2)| e^{-ik_\gamma R_1}|\Psi_a(R_1, R_2)> \quad (6)$$

The values of energy, accepted by vibration and rotational degrees of freedom of the molecule are as follows:

$$\varepsilon_{vib} \approx v\hbar\omega = R_{om}(m_2/m_1),$$
$$\varepsilon_{rot} \approx BJ^2 = R_{om}(m_2/m_1). \quad (7)$$

The simple adequate model for definition of the rotational motion is the rigid rotator approximation. In this approximation the wave functions with definite values of quantum numbers J,K are the eigen functions of the angle momentum operator, i.e.:

$$\psi(R_1, R_2) = Y_{J,K}(\theta, \varphi). \quad (8)$$

In a case of the vibration motion the wave functions with definite value of the vibration quantum number are numerically found by

solving the corresponding Schrödinger equation with potential function, choice of which was discussed above. The simple approximation is surely the harmonic oscillator onee. The harmonic oscillator wave functions were used for estimating matrix elements of the vibration-nuclear transitions in ref. [4]. In general the matrix element of the vibration-rotation-nuclear transition can be written as follows:

$$M_{J_b,K_b;J_a,K_a}^{v_b,v_a} = (4\pi)^{1/2}[(2J_a+1)(2J_b+1)]^{1/2}(-1)^{K_b}$$

$$\sum_{l=|J_b-J_a|}^{J_a+J_b} i^l \{2l+1\}^{1/2} <\Psi_{v_b}|(\pi/2a)^{1/2} J_{l+1/2}(a)|\Psi_{v_a}>$$

$$\begin{pmatrix} J_a & J_b & l \\ 0 & 0 & 0 \end{pmatrix} \sum_{m=-l}^{+l} Y_{lm}^* \begin{pmatrix} J_a & J_b & l \\ k_a & -k_b & m \end{pmatrix}$$

$$a = (E_\gamma^{(o)}/\hbar c)(m_2/M)R^*(1+Q/[(m)^{1/2}R^*] \quad (9)$$

Here $Q = (R-R_o)(m)^{1/2}$, $m = m_1 m_2/M$ is the reduced mass of the molecule, m_1 and m_2 are the masses of nuclei. The co-ordinate of mass centre of the first nucleus relatively the molecule mass centre is defined by expression:

$$R_I = -(m_2/M)R = -(m_2/M)[R_o + Q/(m)^{1/2}] = -(m_2/M)R_o - (m_2/m_1 M)^{1/2}Q$$

The corresponding probability can be written in the following form:

$$P_{J_b J_a}^{v_b v_a} = (2J_b+1)$$

$$\sum_{l=|J_b-J_a|}^{J_a+J_b} \{2l+1\} |<\Psi_{v_b}|(\pi/2a)^{1/2} J_{l+1/2}(a)|\Psi_{v_a}>|^2 \cdot$$

$$\begin{pmatrix} J_a & J_b & l \\ 0 & 0 & 0 \end{pmatrix}^2 \quad (10)$$

Our new approach in in construction of the final potential function as a sum of a few potentyial curves. Each diatomic potential curve dimer is approximated by three functions corresponding to different portions of it. As in Ref. [10], the first portion is approximated by the known perturbed Morse oscillator function:

$$U(R) = V_e\left(y^2 + \sum_{n=4}^{\infty} b_n y^n\right),$$

$$y = 1 - \exp[-\rho(R - R_e)], \quad (11)$$

where R, R_e- and equilibrium internuclear internuclear distance;V_e, ρ, b_n - the parameters of the Morse oscillator function.

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Often in the middle of the potential curve (it is experimentally investigated range of vibrational quantum numbers) it is usuaaly used the potential of the Rydberg-Klein-Rees (look for example [10-15,18]). This potential curve has not the analytical form, and it is built as a set of R_{min} and R_{max} classical turning points for experimental study of vibrational energy levels. Insit of it in our new scheme we apply the Simons-Parr-Finlan molecular potential which looks as follows [15]:

$$U(r) = B_0[(r-r_e)/r]^2\{1 + \sum_n b_n[(r-r_e)/r]^n\} \quad (12a)$$

or introducing $x = r - r_0$:

$$U(r) = B_0[x/(x+r_0)]^2\{1 + \sum_n b_n[x/(x+r_0)]^n\} \quad (12b)$$

where the coefficients b_i are linked with corresponding molecular constants [14].

Finally, the plot of the potential curve for large values of the internuclear distance is approximated by the standard function:

$$U(R) = D_e - \sum \frac{C_n}{R^n} - \Delta U_{обм}(R), \qquad (13)$$

where D_e - experimental value of dissociation energy; C_n – the function parameters (6); n = 3-8. Let us note that the model (11)-(13) is obviously more exact and consistent in comparison with a simple harmonic oscillator one. As an application it was carried out computing the rubidium dimers (Rb2, KRb) diatomics spectral parameters. The results of calculation of molecular constants (cm⁻¹) for the $X^1\Sigma^+$ state of the KRb dimer are presented in table 1 tohether with experimental data [10,19,20] and theoretical data [10,11] obtained with using the Morse- Rydberg - Klein - Rees (M-RKR) method.

Table 1

The molecular constants (cm⁻¹) for the $X^1\Sigma^+$ state of the KRb dimer: Experimantal data – Exp; Theory: a- [10]; b- our data

KRb	$X^1\Sigma^+$		
	Th: a	Th: b	Exp
ω_e	75,846	75,844	75,842
$\omega_e x_e$	0,230	0,230	0,230
$\omega_e y_e$	–3,7(–4)	–3,8(–4)	–3,9(–4)
$\omega_e z_e$	–3,7(–6)	–3,5(–6)	– 3,1(–6)
B_e	0,03815	0,03812	0,03813
α_e	1,21(–4)	1,20(–4)	1,20(–4)
γ_e	–7,3(–7)	–7,3(–7)	–7,4(–7)
D_e	3,85(– 8)	3,85(–8)	3,86(–8)
H_e	3,7(–14)	3,7(–14)	3,7(–14)

Table 2 contains the results of calculation of molecular constants (cm⁻¹) for the $B^1\Pi$ (b) state of the KRb dimer

Table 2

The molecular constants (cm⁻¹) for for the $B^1\Pi$ (b) state of the KRb dimer: Experimantal data – Exp; Theory -our data

KRb	$B^1\Pi$	
	Theory	Exp
ω_e	61,258	61,256
$\omega_e x_e$	0,2095	0,2089
$\omega_e y_e$	2,88(– 3)	2,87(– 3)
$\omega_e z_e$	–1,034(–4)	–1,031(–4)
B_e	0,03287	0,03288
α_e	7,54(– 5)	7,41(– 5)
γ_e	–1,12(– 5)	–1,13(–5)
D_e	3,75(– 8)	3,79(–8)
H_e	5,5(– 14)	5,7(–14)

Tables 3 and 4 contains the same data for states of the rubidium dimer for the $^1\Sigma^+_g$ and $(1)^1\Pi_u(B)$ states.

Table 3

The molecular constants (cm⁻¹) for the $^1\Sigma^+_g$ state of the Rb2 dimer: Experimantal data – Exp; Theory: a- [11]; b- our data

	[16]	Our data	Exp
ω_e	31,4883	31,4884	31,4880
$\omega_e x_e$	–0,1140(–1)	– 0,1142(–1)	–0,1144(–1)
$\omega_e y_e$	–4,255(–4)	– 4,263(–4)	–4,269(–4)
$\omega_e z_e$	7,20(–7)	7,31(–7)	7,40(–7)
B_e	0,13433(–1)	0,13435(–1)	0,13431(–1)
α_e	–1,449(–6)	– 1,468(–6)	–1,485(–6)
γ_e	–4,136(–7)	– 4,132(–7)	–4,122(–7)

Table 4

The molecular constants (cm⁻¹) for the (1)¹Π_u(B) state of the Rb2 dimer: Experimantal data – Exp; Theory: our data

Rb_2	Theory	Exp
ω_e	47,471	47,470
$\omega_e x_e$	0,1431	0,1430
$\omega_e y_e$	$-8,351(-7)$	-
B_e	0,19529(-1)	0,19523(-1)
α_e	1,02(-4)	1,00(-4)
γ_e	1,564(-7)	1,561(-7)

Analsysis of the listed data show a physically reasonable agreement beyween thepretical and experimental data. Further we present the accurate data on the probabilities for vibration-rotation-nuclear transitions from state with v_a=0, J_a=0 and state v_a=1, J_a=0 in a case of the emission and absorption spectrum of nucleus ^{127}I ($E^{(0)}_g$ = 203 keV) linked with molecule H^{127}I in the ground electron state X¹S (molecular parameters: R_o=1,61Å, n_e=2309 cm⁻¹, B=6,55cm⁻¹). The recoil energy for this molecule is 0,172 eV. Parameters which define excitation of vibrations and rotations for this molecule because of the recoil, are as follows: a_o=1.30 and e_o=5.29×10⁻² It should be noted also that a width of the gamma lines are corresponding to temperature T=300K. In figure 1 we present the calculated spectrum of emission and adsorption of nucleus ^{127}I in the H^{127}I .
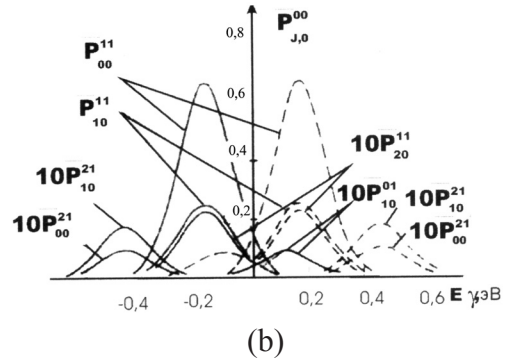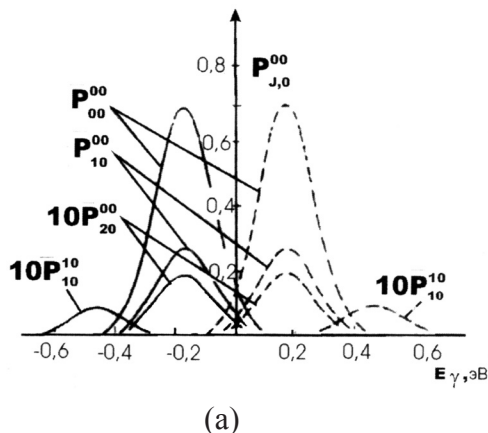
(b)

Fig. 1. Computed emission (solid curve) and absorption spectrum of nucleus ^{127}I ($E^{(0)}_g$ = 203 KeV) in the molecule H^{127}I. Initial state of molecule: a). above n_a=0, J_a=0 and b). below n_a=1, J_a=0 (our data)

We have made comparison of the corresponding vibration-rotation-nuclear transition parobailities from state with v_a=0, J_a=0 and state v_a=1, J_a=0 in a case of the emission and absorption spectrum of nucleus ^{127}I ($E^{(0)}_g$ = 203 keV) in the H^{127}I for different approximations of the for potential curves: the harmonic oscillator [4], the Dunham model [5,7] and presented approach. The values for probabilities, calculated within the present approach and Dunham model for potential curve [7,8], differ from the corresponding ones, calculated within the harmonic oscillator approximation [1], in average on 5-20%. A direct experimental observation of the cooperstive electron-ganna-nuclear effects represents a great fundamental interest. Finally let us note that the presented theory is related to usual molecular systems. At the same time in the last years a great attention is turn to the exotic (hadronic) atomic and molecular systems such pionic and kaonic atoms and molecules. The difference between the usual and exotic molecules at the theoretical level is obviously provided by using the Schrodinger equation in a case of usual molecules and the Klein-Gordon-Fock equation for the pionic and kaonic systems. Taking into accout the results of the last two decades on succseful solutions of the Klein-Gordon-Fock equation with the difeerent (for example, Morse etc) [18] potentials our theory is naturally generalized on a case of exotic diatomic molecules. All theoretical positions are remained the same. Simulteniuosly it is self-undrestood that the relatively quick radiative processes with

(a)

chartacteristic life less than the negative pion and kaon lifetime ($\sim 10^{-8}$s) are of a direct theoretical and practical interest.

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Abstract

It is proposed a new approach to construction of the potential function of diatomic molecules as a sum of the known perturbed Morse oscillator function, the Simons-Parr-Finlan molecular potential in the middle of the potential curve, function of the $-C_n/R^n$ type at the large internuclear distances. Within this approach it is presented a precise scheme for computing the molecular spectral parameters, namely, vibrational, rotational, centrifugal constants for the electronic states of diatomics. As application it was carried out calculation of the of molecular constants (cm^{-1}) for the $X^1\Sigma^+$ $B^1\Pi$ states of the KRb dimer and rubidium dimer and performed further comparison with experimental data. Within consistent approach to calculation of the electron-nuclear g transition spectra (set of vibration-rotational satellites in molecule) of molecule there are obtained the estimates for vibration-rotation-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{127}I $(E_g^{(0)} = 203$ keV$)$ in the molecule of $H^{127}I$ for different approximations of the for potential curves: the hadmonic oscillator, the Dunham model and presented approach.

Key words: electron-g-nuclear transition spectrum, molecules, spectral parameters

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НОВЫЙ КВАНТОВЫЙ ПОДХОД К ОПРЕДЕЛЕНИЮ МОЛЕКУЛЯРНЫХ СПЕКТРАЛЬНЫХ КОНСТАНТ И ВЕРОЯТНОСТЕЙ КООПЕРАТИВНЫХ КОЛЕБАТЕЛЬНО-ВРАЩАТЕЛЬНО-ЯДЕРНЫХ ПЕРЕХОДОВ В СПЕКТРАХ ДВУХАТОМНЫХ И АДРОННЫХ МОЛЕКУЛ

Резюме

Предлагается новый подход к построению потенциальной функции двухатомных молекул в виде суммы известного возмущенной функции осциллятора Морзе, молекулярного потенциала Simons-Паppа-Finlan в средней части потенциальной кривой, функции типа $-C_n/R^n$ при больших межъядерных расстояниях. В рамках этого подхода развита прецизионная схема вычисления молекулярных спектральных параметров, а именно колебательных, вращательных, центробежных постоянных для электронных состояний двухатомных молекул. В качестве приложения проведено вычисление молекулярных констант $(см^{-1})$ для состояний $X^1\Sigma^+$ $B^1\Pi$ димера KRb и димера рубидия и выполнено сравнение с экспериментальными данными. В рамках последовательного подхода к расчету спектров электронно-гамма-ядерных переходов (набор колебательно-вращательных спутников в молекуле) в молекуле получены оценки для колебательно-

вращательных-ядерных вероятностей переходов в случае испускания и поглощения спектра ядро ^{127}I ($E^{(0)}_g = 203$ keV)) в молекуле $H^{127}I$ для различных приближений для потенциальных кривых: модели гармонического осциллятора, модели на основе потенциала Данхэм и предложенного в работе нового подхода.

Ключевые слова: спектр электрон- g -ядерных переходов, молекулы, спектральные параметры

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НОВИЙ КВАНТОВИЙ ПІДХІД ДО ВИЗНАЧЕННЯ МОЛЕКУЛЯРНИХ СПЕКТРАЛЬНИХ КОНСТАНТ І ІМОВІРНОСТЕЙ КООПЕРАТИВНИХ КОЛИВАЛЬНО- ОБЕРТАЛЬНО -ЯДЕРНИХ ПЕРЕХОДІВ У СПЕКТРІ ДВОАТОМНИХ І АДРОННИХ МОЛЕКУЛ

Резюме

Пропонується новий підхід до побудови потенційної функції двохатомних молекул у вигляді суми відомого обуреної функції осцилятора Морзе, молекулярного потенціалу Simons-Парра-Finlan в середній частині потенційної кривої, функції типу $-C_n / R^n$ при великих меж'ядерних відстанях. В рамках цього підходу розвинена прецизійна схема обчислення молекулярних спектральних параметрів, а саме коливальних, обертальних, відцентрових постійних для електронних станів двохатомних молекул. Як додаток проведено обчислення молекулярних констант (**см-^{1}**) для станів $X^1\Sigma^+$ $B^1\Pi$ димера KRb і димера рубідію і виконано порівняння з експериментальними даними. В рамках послідовного підходу до розрахунку спектрів електронногамма-ядерних переходів (набір колебательно-обертальних супутників в молекулі) в молекулі отримані оцінки для колебательно-обертальних-ядерних ймовірностей переходів в разі випускання і поглинання спектра ядро ^{127}I ($E^{(0)}_g = 203$ keV) в молекулі $H^{127}I$ для різних наближень для потенційних кривих: моделі гармонійного осцилятора, моделі на основі потенціалу Данхем і запропонованого в роботі нового підходу.

Ключові слова: спектр електрон- g -ядерних переходів, молекули, спектральні параметри