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ОПТИЧНІ, ОПТОЕЛЕКТРОННІ І РАДІАЦІЙНІ СЕНСОРИ

SENSING COOPERATIVE ELECTRON-GAMMA-NUCLEAR EFFECT IN MULTIATOMIC MOLECULES AND ITS APPLICATION

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SENSING COOPERATIVE ELECTRON-GAMMA-NUCLEAR EFFECT IN MULTIATOMIC MOLECULES AND ITS APPLICATION

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Abstract. Nowadays, the cooperative spectral effects for polyatomic molecules in the external field of laser radiation are of great interest for sensor and quantum electronics, molecular spectroscopy. When a nucleus in a molecule absorbs or emits a photon, then it is possible changing the electron, vibrational and rotational energy of the molecule, and then the so-called cooperative electron-vibrational-rotational-nuclear transitions take place. The spectrum of a molecule contains a set of electron-vibrational-rotational-nuclear satellites, the appearance of which is caused by a change in the state of a molecular system interacting with a photon. This paper presents the first quantitative data on the probability of vibrational -nuclear transitions in the case of the radiation spectrum and absorption of the ^{186}Re nucleus (E = 186.7 keV) in the ReO_4 molecule. It seems that the cooperative electron-gamma-nuclear effect in the spectra of polyatomic molecules can be used as a basis for the creation of new techniques and practical implementations of molecular sensors.

Keywords: sensor, multiatomic molecules, electron-gamma-nuclear effect

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ДЕТЕКТУВАННЯ КООПЕРАТИВНОГО ЕЛЕКТРОН-ГАММА-ЯДЕРНОГО ЕФЕКТУ ДЛЯ БАГАТОАТОМНИХ МОЛЕКУЛ ТА ЙОГО ЗАСТОСУВАННЯ

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Анотація. За теперішнього часу величезний інтерес для сенсорної та квантової електроніки, молеклярної спектроскопії тощо викликає вивчення кооперативних спектральних ефектів в багатоатомних молекулах у зовнішньому полі лазерного випромінювання. Коли ядро в молекулі поглинає або випромінює фотон, то є можливим змінення електронної, коливальної та обертальної енергії молекули, і далі мають місце так звані кооперативні електронно-коливально-обертально-ядерні переходи. Спектр молекули містить набір електрон-коливально-обертально-ядерних супутників, поява яких зумовлена зміненням стану молекуклярної системи, що взаємодіє з фотоном. В даній роботі представлені перші кількісні дані щодо ймовірностей коливально-ядерних переходів у випадку спектру випромінювання та поглинання ядра ^{186}Re (E = 186.7 кеВ) у молекулі ReO$_4$. Представляється, що кооперативний електрон-гамма-ядерний ефект у спектрах багатоатомних молекул може бути використаний як основа для створення нових методик та практичних реалізацій молекулярних сенсорів.

Ключові слова: сенсор, багатоатомні молекули, електрон-гамма-ядерний ефект

ДЕТЕКТИРОВАНИЕ КООПЕРАТИВНОГО ЭЛЕКТРОН-ГАММА-ЯДЕРНОГО ЭФФЕКТА ДЛЯ МНОГОАТОМНЫХ МОЛЕКУЛ И ЕГО ПРИМЕНЕНИЕ

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Аннотация. В настоящее время огромный интерес для сенсорной и квантовой электроники, молекулярной спектроскопии и т.д. вызывает изучение кооперативных спектральных эффектов в многоатомных молекулах во внешнем поле лазерного излучения. Когда ядро в молекуле поглощает или излучает фотон, то становится возможным изменение электронной, колебательной и вращательной энергии молекулы, и дальше имеют место так называемые кооперативные электронно-колебательно-вращательно-ядерные переходы. Спектр молекулы содержит набор электрон-колебательно-вращательно-ядерных спутников, появление которых обусловлено изменением состояния молекуклярнои системы, взаимодействующей с фотоном. В данной работе представлены первые количественные данные о вероятностях колебательно-ядерных переходов в спектре излучения и поглощения ядра ^{186}Re (E = 186.7 кэВ) в молекуле ReO$_4$. Представляется, что кооперативный электрон-гамма-ядерный эффект в спектрах многоатомных молекул может быть использован как основа для создания новых методик и практических реализаций молекулярных сенсоров.

Ключевые слова: сенсор, многоатомные молекулы, электронно-гамма-ядерный эффект

1. Introduction

Currently, one of the promising areas of a sensor electronics, atomic, nuclear and molecular spectroscopy and physics is creating atomic/molecular sensors to detect different compounds or phenomena. There are various types of molecular sensors, and, as a rule, the principles of their work are based on certain physical or chemical properties and phenomena (c.g., [1-20]). Being investigated the possibility of creating a molecular sensor of the concept of "electronic nose" – type analyzer vapor substances in the air is based on organic sensory polymer composites. A great interest attracts study of the cooperative molecular spectral effects for multiatomic molecules in an external laser radiation field [21-31]. Really, any alteration of the molecular state must be manifested in the quantum transitions, for example, in a spectrum of the γ -radiation of a nucleus of some molecular system. When the nucleus in the molecule absorbs or emits a photon, then it is possible changing the electronic, vibrational and rotational energy of the molecule, and therefore electronic-vibrational-rotational-nuclear transitions occur. Of course, the intensity of additional satellites is determined by the probability of such composite transitions for the core in a molecule" system. By changing the population of excited states of an atom or molecule by laser radiation, it is possible, firstly, to control the intensity of cooperative transitions and, secondly, to create new transitions that are shifted to the long-wavelength side relative to the absorption line and to the short-wavelength side relative to the gamma-emission line. In fact it is possible to transfer a part of the nuclear energy to an atom or molecule under radiating (absorption) the γ quanta by a nucleus (c.g., [21-31]). A spectrum contains a set of the electron-vibration-rotation satellites, which are due to an alteration of the state of system interacting with photon. The mechanism of forming satellites in the molecule is connected with a shaking of the electron shell resulting from the interaction between a nucleus and γ quantum.

Studying the co-operative dynamical phenomena due to interaction between atoms, ions, molecule electron shells and nuclei nucleons is now one of the quickly developing directions in a modern molecular spectroscopy and quantum electronics [27, 28]. A consistent quantum- mechanical approach to calculation of the electron-nuclear γ transition spectra of a nucleus in the multiatomic molecules has been earlier proposed [23-28]. It generalizes the well-known approach [21, 22] by Letokhov and Minogin, who firstly indicated on the rich cooperative electron-gamma-molecular quantum physics. Estimates of the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{188}Os in the OsO_4 and ^{191}Ir in the IrO_4 were earlier listed [23-26]. In this paper we present the first accurate data on the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of the nucleus ^{186}Re ($E^{(0)}_\gamma = 186.7$ keV) in the ReO_4. We believe that the cooperative electron-gamma-nuclear effect in spectra of multiatomic molecules can be used as a basis for creating new methodises and practical realizations of effective molecular sensors.

2. Theoretical treatment of cooperative electron-gamma-nuclear effect in multiatomic molecule

As the method of computing is earlier presented in details [22-24], here we consider the key topics only. Hamiltonian of interaction of the gamma radiation with a system of nucleons for the first nucleus is expressed through the co-ordinates of nucleons r_n' in a system of the mass centre of one nucleus: $H(r_n) = H(r_n')\exp(-ik_\gamma u)$, where k_γ is a wave vector of the γ quantum; u is the shift vector from equality state (coinciding with molecule mass centre) in a system of co-ordinates in the space. The matrix element for transition from the initial state "a" to the final state "b" is presented as:

$$< \Psi_b^* \, | \, H \, | \, \Psi_a > \bullet < \Psi_b^* \, | \, e^{-ik_\gamma u} \, | \, \Psi_a > \qquad (1)$$

where a and b is a set of quantum numbers, which define the vibrational and rotational states before and after interaction (with γ quantum). The first multiplier in (1) is defined by the γ transition of nucleus and is not dependent on an internal structure of molecule in a good approximation. The 2nd multiplier is the matrix element of transition from the initial state "a" to the final state "b":

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

$$(2)$$

The expression (2) gives a general formula for calculating the probability of changing the internal state of molecule during absorption or emitting γ quantum by a nucleus. It determines an intensity of the corresponding γ-satellites. Their positions are fully determined as:

$$E_\gamma = E_\gamma^0 \pm R + \hbar k_\gamma v \pm (E_b - E_a)$$

Here M is the molecule mass, v is a velocity of molecule before interaction of nucleus with γ quantum; E_a and E_b are the energies of the molecule before and after interaction; E_γ is an energy of nuclear transition; R is an energy of recoil:

$$R = [(E_\gamma^{(0)})]^2 / 2Mc^2.$$

One can suppose that only single non-generate normal vibration (vibration quantum $\hbar\omega$) is excited and initially a molecule is on the vibrational level $v_a = 0$. If we denote a probability of the corresponding excitation as $P(v_b, v_a)$ and use expression for shift u of the γ-active nucleus through the normal co-ordinates, then an averaged energy for excitation of the single normal vibration is as follows [22,23]:

$$\overline{E}_{vib} = \sum_{v=0}^{\infty} \hbar\omega(v + \tfrac{1}{2})\overline{P}(v,0) - \hbar\infty/2 = \sum_{v=0}^{\infty} \hbar\omega(v + \tfrac{1}{2})P(v,0) - \hbar\omega/2 =$$

$$= \sum_{v=0} \hbar\omega(v + \tfrac{1}{2})\frac{z^v}{v!}e^{-z} - \frac{\hbar\omega}{2} = \frac{1}{2}R\left(\frac{M-m}{m}\right), \quad (3)$$

where $z = (R/\hbar\omega)[M - m/m]\cos^2\vartheta$, and m is the mass of γ-active nucleus, ϑ is an angle between nucleus shift vector and wave vector of γ-quantum and line in $\overline{E}_{vib}$ means averaging on orientations of molecule (or on angles ϑ). To estimate an averaged energy for excitation of the molecule rotation, one must not miss the molecule vibrations as they provide non-zeroth momentum $L = k_v u \sin\vartheta$, which is transferred to a molecule by γ-quantum. Assuming that a nucleus is only in the single non-generate normal vibration and vibrational state of a molecule is not changed $v_a = v_b = 0$, one could evaluate an averaged energy

for excitation of the molecule rotations as follows:

$$\overline{E}_{rot} = \left\langle \overline{BL^2} \right\rangle = BL_\gamma^2 \left\langle u^2 \right\rangle \overline{\sin^2\vartheta} = \tfrac{1}{2}R(B/\hbar\omega)[(M-m)/m]$$

$$(4)$$

A shift u of the γ-active nucleus can be expressed through the normal co-ordinates $Q_{s\sigma}$ of a molecule:

$$u = \frac{1}{\sqrt{m}}\sum_{s\sigma} b_{s\sigma}Q_{s\sigma} \qquad (5)$$

where m is a mass of the γ-active nucleus; components of the vector $b_{s\sigma}$ of nucleus shift due to the σ-component of "s" normal vibration of a molecule are the elements of matrix b [27, 32-37]; it realizes the orthogonal transformation of the normal co-ordinates matrix Q to matrix of masses of the weighted Cartesian components of the molecule nuclei shifts q. Further $M(b,\alpha)$ is rewritten as multiplying matrix elements on molecule normal vibration, which takes contribution to a shift of γ-active nucleus:

$$M(b,a) = \prod_s \left\langle v_s^b \,\Big|\, \prod_\sigma \exp(-ik_\gamma b_{s\sigma}Q_{s\sigma}/\sqrt{m})v_s^a \right|\right\rangle. \quad (6)$$

Usually wave functions of a molecule can be written for non-degenerate vibration as:

$$|v_s\rangle = \Phi_{vs}(Q_s),$$

for double degenerated vibration as

$$|v_s\rangle = (v_s + 1)^{-\tfrac{1}{2}} \sum_{vs\sigma_1, vs\sigma_2, vs_s} \Phi_{v_{s\sigma_1}}(Q_{s\sigma_1})\Phi_{v_{s\sigma_2}}(Q_{s\sigma_2})$$

(where $v_{s\sigma_1} + v_{s\sigma_2} = v_s$) and analogously for triple degenerate vibration. In the simple approximation function $\Phi v_{s\sigma}(Q_{s\sigma})$ can be chosen in a form of the linear harmonic oscillator one. More exact calculating requires a numerical determination of these functions. Taking directly the wave functions $|v_s^\alpha\rangle$ and $|v_s^b\rangle$, determination of the matrix element (6) is reduced to calculation of the matrix elements on each component σ of the normal vibration.

3. Results and conclusions

Below we present the advanced data on the vibration-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{186}Re ($E^{(0)}_\gamma$ = 186.7 keV) in the molecule ReO$_4$. Note that the main difficulty during calculating (6) is connected with definition of the values $b_{s\sigma}$ of the normalized shifts of γ-active decay. It is known that if a molecule has the only normal vibration of the given symmetry type, then the corresponding values of $b_{s\sigma}$ can be found from the well known Eckart conditions, normalization one and data about the molecule symmetry. For several normal vibrations of the one symmetry type, a definition of $b_{s\sigma}$ requires solving the secular equation for molecule |GF-λ E|=0. We have used the results of advanced theoretical calculating electron structure of the studied system within an advanced relativistic scheme of the density functional method (c.g., [27, 32, 38]). In table 1 we list the results of calculating probabilities of the first several vibration-nuclear transitions in a case of the emission and absorption spectrum of the nucleus ^{186}Re ($E^{(0)}_\gamma$ = 186.7 keV) in the molecule ReO$_4$.

In conclusion let us note that by changing the population of excited states of an atom or molecule by laser radiation, it is possible, firstly, to control the intensity of cooperative gamma-transition and, secondly, to create new gamma-transitions that are shifted to the long-wavelength side relative to the absorption line $\left(E_0 + R\right)$ and to the short-wavelength side relative to the gamma-emission line $\left(E_0 - R\right)$.

Table 1

Probabilitites of the vibrational-nuclear transitions in spectrum of the ReO$_4$

Vibration transition $v_3^a, v_4^a - v_3^b, v_4^b$	$\overline{P}$ ($v_3^a, v_4^a - v_3^b, v_4^b$)
0,0 − 0,0	0.74
1,0 − 0,0	0.014
0,1 − 0,0	0.067
1,0 − 1,0	0.68
0,1 − 0,1	0.61

Laser radiation can excite atoms or molecules with a specific projection of the speed of motion in the selected direction (the direction of the light wave), i.e. change the equilibrium distribution of particle velocities at levels associated with the laser field. As it was indicated by Letokhov, one could prepair the excited molecule moving with a velocity $\vec{v}_{pe3}$, which is determined by the optical resonance condition $\vec{k}_0 \vec{v}_{pe3} = w - w_0$, wkere $\vec{k}_0$ is a wave vector of a laser wave, $\vec{v}_{pe3}$ is a frequency of a laser field and w_0 is a frequency of molecular transition.

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SENSING COOPERATIVE ELECTRON-GAMMA-NUCLEAR EFFECT IN MULTIATOMIC MOLECULES AND ITS APPLICATION

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Summary

One of the promising areas of sensor electronics, molecular spectroscopy and physics is the creation of molecular sensors for the detection of various compounds or phenomena, and, as a rule, the principle of operation of a molecular sensor is based on certain physical or chemical properties or effects. Nowadays, the cooperative spectral effects for polyatomic molecules in the external field of laser radiation are of great interest. When a nucleus in a molecule absorbs or emits a photon, then it is possible changing the electron, vibrational and rotational energy of the molecule, and then the so-called cooperative electron-vibrational-rotational-nuclear transitions take place. The spectrum of a molecule contains a set of electron-vibrational-rotational-nuclear satellites, the appearance of which is caused by a change in the state of a molecular system interacting with a photon. This paper presents the first quantitative data on the probability of vibrational -nuclear transitions in the case of the radiation spectrum and absorption of the ^{186}Re nucleus (E = 186.7 keV) in the ReO_4 molecule. It seems that the cooperative electron-gamma-nuclear effect in the spectra of polyatomic molecules can be used as a basis for the creation of new techniques and practical implementations of molecular sensors.

Keywords: chemical sensor, multiatomic molecules, electron-gamma-nuclear effect

ДЕТЕКТУВАННЯ КООПЕРАТИВНОГО ЕЛЕКТРОН-ГАММА-ЯДЕРНОГО ЕФЕКТУ ДЛЯ БАГАТОАТОМНИХ МОЛЕКУЛ ТА ЙОГО ЗАСТОСУВАННЯ

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Реферат

Однією з перспективних областей сенсорної електроніки, молекулярної спектроскопії є створення молекулярних датчиків для виявлення різних сполук або явищ, причому, як правило принцип роботи того чи іншого молекулярного сенсора базується на певних фізичних чи

хімічних властивостях або ефектах. За теперішнього часу величезний інтерес викликають кооперативні спектральні ефекти для багатоатомних молекул у зовнішньому полі лазерного випромінювання. Коли ядро в молекулі поглинає або випромінює фотон, то є можливим змінення електронної, коливальної та обертальної енергії молекули, і далі мають місце так звані кооперативні електронно-коливально-обертально-ядерні переходи. Спектр молекули містить набір електрон-коливально-обертально-ядерних супутників, поява яких зумовлена зміненням стану молекуклярної системи, що взаємодіє з фотоном. В даній роботі представлені перші кількісні дані щодо ймовірностей коливально-ядерних переходів у випадку спектру випромінювання та поглинання ядра ^{186}Re (E = 186.7 кеВ) у молекулі ReO_4. Представляється, що кооперативний електрон-гамма-ядерний ефект у спектрах багатоатомних молекул може бути використаний як основа для створення нових методик та практичних реалізацій молекулярних сенсорів.

Ключові слова: сенсор, багатоатомні молекули, електрон-гамма-ядерний ефект