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SPECTROSCOPY OF COOPERATIVE ELECTRON-γ- NUCLEAR EFFECTS IN MULTIATOMIC MOLECULES: MOLECULE XY_4

The consistent quantum approach to calculating the electron-nuclear γ transition spectra (a set of the vibration-rotational satellites in a molecule) of a nucleus in the multiatomic molecules is used to get the accurate spectroscopic 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 of ReO_4. the main difficulty during calculating corresponding matrix elements 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 Eccart conditions, normalization one and data about the molecule symmetry.

1. Introduction

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. It is well known that it is possible the transfer of part of a nuclear energy to atom or molecule under radiating (absorption) the γ quanta by a nucleus (c.f.[1-36]). 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. A 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. This paper is going on our studying the co-operative dynamical phenomena (c.f.[6б7]) due the interaction between atoms, ions, molecule electron shells and nuclei nucleons. 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 [2-5]. It generalizes the well known Letokhov-Minogin model [2]. 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 listed . Here 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.

2. The electron-nuclear γ transition spectra of nucleus in multi-atomic molecule

As the method of computing is earlier presented in details [2-6], here we consider only by the key topics. Hamiltonian of interaction of the gamma radiation with a system of nucleons for the first nucleus can be expressed through the coordinates of nucleons r_n' in a system of the mass centre of one nucleus [2,3]:

$$H(r_n) = H(r_n')\exp(-k_{\gamma}u),$$

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 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 :

$$< \Psi_b^* \mid H \mid \Psi_a > \bullet < \Psi_b^* \mid \hat{a}^{-k_\gamma u} \mid \Psi_a > \qquad (1)$$

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 second multiplier is the matrix element of transition from the initial state "a" to the final state "b":

$$M_{ba} \propto \Psi_b^*(r_e) \mid \Psi_a(r_e) >$$

$$\bullet < \Psi_b^*(R_1, R_2) \mid e^{-k_\gamma R_1} \mid \Psi_a(R_1, R_2) > \qquad (2)$$

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_{om} is an energy of recoil:

$$R_{om} = [(E_\gamma^{(o)}]^2 / 2Mc^2.$$

One can suppose that only single non-generated 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:

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

$$= \sum_{v=0}^{\infty} \hbar\omega\left(v + \tfrac{1}{2}\right)P(v,0) - \hbar\omega/2 =$$

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

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 $L = k_v \sin\vartheta$, which is transferred to a molecule by γ-quantum. In supposing that a nucleus is only in the single non-generated 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:

$$\overline{E}_{rot} = \left\langle \overline{BL^2} \right\rangle = Bk_\gamma^2 \left\langle u^2 \right\rangle \overline{\sin^2\vartheta} = \tfrac{1}{2}R(B/\hbar\omega)[(M-m)/m] \qquad (4)$$

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 [2]; 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. According to (2), the matrix element can be written as multiplying the matrix elements on molecule normal vibration, which takes contribution to a shift of the γ-active nucleus:

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

It is obvious that missing molecular rotations means missing the rotations which are connected with the degenerated vibrations. Usually wave functions of a molecule can be written for non-degenerated vibration as:

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

for double degenerated vibration as

$$|v_s\rangle=(v_s+1)^{-1/2}\sum_{v\sigma_1,v\sigma_2,v\sigma_3}\Phi_{v_{s\sigma_1}}(Q_{s\sigma_1})\Phi_{v_{s\sigma_2}}(Q_{s\sigma_2})$$

where $v_{s\sigma_1}+v_{s\sigma_2}=v_s$ and analogously for triple degenerated 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 $|v_s^a\rangle$ and $|v_s^b\rangle$, calculating the matrix element (6) is reduced to a definition of the matrix elements on each component **γ** 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 ^{191}Ir ($E^{(0)}_\gamma$ = 82 keV) in the molecule IrO_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 Eccart 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 $|GF-\lambda E|=0$. We have used the results of advanced theoretical calculating electron structure of the studied system within an advanced relativistic scheme of the X_α- scattered waves method (see details in Refs.[21-23]). In table 1 we present the results of calculating probabilities of the first several vibration-nuclear transitions in a case of the emission and absorption spectrum of nucleus the nucleus ^{186}Re ($E^{(0)}_\gamma$ = 186.7 keV) in the ReO_4.

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

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SPECTROSCOPY OF COOPERATIVE ELECTRON-γ-NUCLEAR EFFECTS IN MULTIATOMIC MOLECULES: MOLECULE XY_4

Summary

The consistent quantum approach to calculating the electron-nuclear γ transition spectra (a set of the vibration-rotational satellites in a molecule) of a nucleus in the multiatomic molecules is used to get the accurate spectroscopic 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 of ReO_4. the main difficulty during calculating corresponding matrix elements is connected with definition of the values $b_{s\gamma-}$ 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 $b_{s\gamma}$ can be found from the well known Eccart conditions, normalization one and data about the molecule symmetry.

Key words electron-nuclear γ transition spectra, vibration-nuclear transition probabilities

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СПЕКТРОСКОПИЯ КООПЕРАТИВНЫХ ЭЛЕКТРОН-ГАММА-ЯДЕРНЫХ ЭФФЕКТОВ В МНОГОАТОМНЫХ МОЛЕКУЛАХ: МОЛЕКУЛА XY_4

Резюме

Последовательный квантовый подход к вычислению спектров электронно-гамма-ядерных переходов (набора колебательно-вращательных сателлитов в молекуле) в многоатомных молекулах применен к определению спектроскопических данных о вероятностях колебательно-

ядерных переходов при излучении и поглощении ядра ^{186}Re ($E^{(0)}_{\gamma}$= 186.7 кэВ) в молекуле ReO_4. Основная трудность при оценке соответствующих матричных элементов связана с определением значений $b_{s\gamma\text{-}}$ нормированных сдвигов гамма-активного распада. Известно, что если молекула имеет единственное нормальное колебание данного типа симметрии, то соответствующие значения $b_{s\gamma\text{-}}$ могут быть найдены из хорошо известных условий Эккарта, условия нормировки и данных о симметрии молекулы.

Ключевые слова: электронно-гамма-ядерный спектр, вероятность колебательно-ядерных переходов

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СПЕКТРОСКОПІЯ КООПЕРАТИВНИХ ЕЛЕКТРОН-ГАММА-ЯДЕРНИХ ЕФЕКТІВ В БАГАТОАТОМНИХ МОЛЕКУЛАХ: МОЛЕКУЛА XY_4

Резюме

Послідовний квантовий підхід до обчислення спектрів електронно-гамма-ядерних переходів (набору колебательно-обертальних сателітів в молекулі) в багатоатомних молекулах застосований до визначення спектроскопічних даних про ймовірності колебательно-ядерних переходів при випромінюванні і поглинанні ядра ^{186}Re ($E^{(0)}_{\gamma}$= 186.7 кеВ) в молекулі ReO4. Основні труднощі при оцінці відповідних матричних елементів пов’язана з визначенням значень $b_{s\gamma\text{-}}$ – нормованих зрушень гамма-активного розпаду. Відомо, що якщо молекула має єдине нормальне коливання даного типу симетрії, то відповідні значення $b_{s\gamma\text{-}}$ – можуть бути знайдені з добре відомих умов Еккарта, умови нормування і даних про симетрію молекули.

Ключові слова: електрон-гамма-ядерний спектр, ймовірність коливально-ядерних переходів