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PACS 23.20.-g, 23.90.+w,
25.20.Dc, 27.70.+q

NUCLEAR EXCITATION BY ELECTRON TRANSITION

A theory of the nuclear excitation by an electron transition (NEET) induced by x-rays is developed on the basis of the strict collision theory. All stages of the process are considered, including the formation of a hole in an inner electronic shell, its decay leading to the excitation of the nucleus, as well as the subsequent filling of the upper level vacancy and the deexcitation of the nucleus. The cross sections are calculated for NEET and the photoabsorption of x-rays near the absorption edge. The results agree with the data of Kishimoto et al. for NEET on ^{197}Au. In addition, we discuss the NEET mechanism of triggering of the 31-year isomer $^{178}Hf^{m2}$ via an intermediate level induced by x-rays. We have shown that the 2% decay acceleration of this isomer declared by Collins et al. is realistic if the nucleus attributes a triaxial shape in the intermediate state, and there exists an additional rotational band with the 13^- level.

K e y w o r d s: nuclear isomers, Hf, NEET, induced nuclear decay, x-rays.

1. Introduction

When the x-ray photon ionizes one of the inner atomic levels, the appearing vacancy mainly decays, by either emitting another x-ray photon or Auger electron. But there is one more, although weak, decay channel, which is called NEET [1]. In this case, an electron from the upper level, when filling the vacancy, emits the virtual photon, which is then absorbed by the nucleus. Such a resonant process becomes possible if the nuclear and atomic transitions have the same multipolarity and closely lying energies. It has been successfully observed for nuclei ^{197}Au [2], ^{189}Os [3–6], and ^{237}Np [7].

The best resonant conditions are provided in ^{197}Au. Here, the electron, passing from the level M_1 ($3s_{1/2}$, 3.425 keV) to the vacant K-level ($1s_{1/2}$, 80.725 keV), gives rise to the transition of nucleus ^{197}Au from the ground state $3/2^+$ to the first excited state $1/2^+$. In both cases, the transitions are of the M1 multipolarity. As to the energy of the nuclear $1/2^+$ level, it is 77.351 keV according to [8] and 77.339 ± 0.003 keV according to the last precision measurements [9].

The corresponding mismatch of the nuclear ($E_0^{(n)}$) and atomic ($E_0^{(a)}$) transition energies, defined as

$$\delta = E_0^{(n)} - E_0^{(a)}, \qquad (1)$$

will be $\delta = 51$ eV if we accept the value of nuclear energy $E_0^{(n)} = 77.351$ keV, whereas $\delta = 39$ eV if $E_0^{(n)} = 77.339$ keV. Kishimoto *et al.* [2], irradiating a golden foil by synchrotron radiation with the narrow bandwidth $\Gamma_s = 3.5$ eV, found that the NEET edge, as a function of the incident x-ray photon energy E, was shifted higher than the K-absorption edge by $\Delta E = 40 \pm 2$ eV and was much steeper. The NEET probability amounted to $P_{\text{NEET}} = 4.5 \times 10^{-8}$.

The early theories of NEET [10–13] have considered only an intermediate stage of the NEET process. Namely, they believed that, in the initial state of the system (atomic electrons + nucleus), there are a vacancy on the lower atomic level and the unexcited nucleus; while, in the final state, there are a vacancy on the upper level and the resonantly excited nucleus. The ionization of the atom, the forthcoming relaxation of the electronic subsystem, and the decay of the excited nucleus were not taken into consideration.

Nevertheless, such an approximation appears to be sufficient for the correct derivation of the NEET probability far from the NEET edge [10, 12]:

$$P_{\text{NEET}} = \left(1 + \frac{\Gamma_f}{\Gamma_i}\right) \frac{E_{\text{int}}^2}{\delta^2 + (\Gamma_i + \Gamma_f)^2/4}, \qquad (2)$$

where Γ_i and Γ_f are the widths of the initial and final atomic hole states, and E_{int}^2 stands for the coupling strength of atomic electrons and the nucleus. But it failed to describe the effect near the NEET edge.

The initial stage of the NEET process, i.e., the K-hole formation caused by an incident x-ray photon, was considered by Tkalya [13] in the framework of quantum electrodynamics. For the description of resonances, the real energies in electron propagators were replaced by their complex values, which corresponds to the infinite values of wave functions at the initial moment $t \to -\infty$ of the collision of an incident x-ray photon with the atom. Moreover, the δ function corresponding to the energy conservation law has been replaced *ad hoc* by a Lorentzian in order to take an attenuation of the atomic and nuclear excited levels into account.

A more strict approach has been proposed in our previous work [14] based on the collision theory. There, we considered all stages of the photo-induced NEET, including the formation of a vacancy in an inner atomic shell, followed by the energy transfer to a nucleus, then the filling of a new highly lying vacancy and, at last, the decay of the nucleus. Both processes NEET and x-ray absorption were studied on the same basis. Unfortunately, we dealt only with the electric multipole transitions.

In this paper we, give a more general description of NEET, including both the electric and magnetic multipole transitions involved in NEET. In addition, we consider NEET on isomer $^{178}\text{Hf}^{m2}$. The main attention is paid to the shape of the NEET cross section $\sigma_{\text{NEET}}(E)$, as well as to a possible decay path of the intermediate nuclear level bypassing the initial isomeric state.

2. Transition Matrix

The unperturbed Hamiltonian of the system (nucleus + atomic electrons + quantized electromagnetic field) is

$$\hat{H}_0 = \hat{H}_{\text{n}} + \hat{H}_{\text{a}} + \hat{H}_{\text{rad}}, \qquad (3)$$

where $\hat{H}_{\text{n}}$, $\hat{H}_{\text{a}}$, and $\hat{H}_{\text{rad}}$ define, respectively, the Hamiltonians of the nucleus, atomic electrons, and the quantized electromagnetic field. In particular,

$$\hat{H}_{\text{rad}} = \sum_{\mathbf{k}} \sum_{\lambda} \hat{a}_{\mathbf{k}\lambda}^+ \hat{a}_{\mathbf{k}\lambda}, \qquad (4)$$

where $\hat{a}_{\mathbf{k}\lambda}^+$ and $\hat{a}_{\mathbf{k}\lambda}$ are the creation and annihilation operators of a photon with the wave vector $\mathbf{k}$ and the polarization λ.

The total Hamiltonian will be $\hat{H} = \hat{H}_0 + \hat{V}$ with the perturbation

$$\hat{V} = \hat{V}_r^{(n)} + \hat{V}_r^{(a)}, \qquad (5)$$

where $\hat{V}_r^{(n)}$ and $\hat{V}_r^{(a)}$ are the interaction operators of the nucleus and atomic electrons with the electromagnetic field:

$$\begin{aligned} \hat{V}_r^{(n)} &= \frac{1}{c} \int d\mathbf{R}(\hat{J}(\mathbf{R})\hat{A}(\mathbf{R})), \\ \hat{V}_r^{(a)} &= \frac{1}{c} \int d\mathbf{r}(\hat{j}(\mathbf{r})\hat{A}(\mathbf{r})), \end{aligned} \qquad (6)$$

$\hat{J}(\mathbf{R})$ and $\hat{j}(\mathbf{r})$ are the 4-dimensional current density operators of the nucleus and atomic electrons, respectively, and $\hat{A}(\mathbf{r})$ is the 4-vector field potential.

The eigenfunctions and the eigenvalues of the unperturbed Hamiltonian $\hat{H}_0$ obey the equation

$$\hat{H}_0 \chi_b = E_b \chi_b. \qquad (7)$$

Let, at the initial moment $t \to -\infty$, the system be described by the wave function

$$\chi_a = |I_i M_i\rangle \Phi_0 |1_{\mathbf{ke}}\rangle, \qquad (8)$$

where the wave function $|I_i M_i\rangle$ describes the initial state of the nucleus with spin I_i and its projection M_i on the quantization axis, Φ_0 is the initial state of the atom, and $|1_{\mathbf{ke}}\rangle$ is the quantized field containing one x-ray photon with the wave vector $\mathbf{k}$ and the polarization $\mathbf{e}$. The corresponding initial energy of the system

$$E_{\text{a}} = W_i^{(n)} + E, \qquad (9)$$

where $W_i^{(n)}$ is the initial energy of the nucleus (for the atom, it is chosen to be zero), and E is the incident photon energy.

At first, the electron absorbs an x-ray photon and flies away with the wave vector $\boldsymbol{\kappa}$ and the kinetic energy ε, by leaving the hole in the i-th atomic level.

Such first intermediate state of the system is described by the wave function

$$|c_1\rangle = |I_i M_i\rangle \Phi_i |\boldsymbol{\kappa}\rangle |0\rangle, \tag{10}$$

where $|0\rangle$ stands for the wave function of the vacuum of the electromagnetic field, Φ_i and $|\boldsymbol{\kappa}\rangle$ are the functions of the atom with the i-th hole and the ejected electron, respectively. The corresponding eigenvalue of the unperturbed Hamiltonian $\hat{H}_0$ is as follows:

$$E_1 = W_i^{(n)} + B_i + \varepsilon. \tag{11}$$

Hereafter, B_i and B_f are the binding energies of the electron in the orbits labeled by i and f.

After that, the electron, by passing down from the f-th orbit into the i-th one, transfers its energy to the nucleus (NEET). The whole system undergoes the transition into the second intermediate state

$$|c_2\rangle = |I_e M_e\rangle \Phi_f |\boldsymbol{\kappa}\rangle |0\rangle \tag{12}$$

with the energy

$$E_2 = W_e^{(n)} + B_f + \varepsilon, \tag{13}$$

where $|I_e M_e\rangle$ and $W_e^{(n)}$ are the wave function and the energy of the excited nucleus. The nuclear and atomic transition energies are $E_0^{(n)} = W_e^{(n)} - W_i^{(n)}$ and $E_0^{(a)} = B_i - B_f$, respectively.

In principle, two decay branches of the state $|c_2\rangle$ are possible: deexcitation of the nucleus and decay of the fth hole. But the decay rate of the atomic holes is by many orders larger than that of the nucleus. In particular, the width of the first excited level for ^{197}Au $\Gamma_n = 2.38 \times 10^{-7}$ eV, while the K-hole width $\Gamma_K = 52$ eV and the M_1-hole width $\Gamma_{M_1} = 14.3$ eV [2]. Thus, at first, there are the electron transitions that lead to the filling of the f-th hole. For brevity, we talk about a single electron transition from an upper level with the binding energy B', followed by the emission of a photon with the energy $\hbar\omega'$.

After the relaxation of the atomic electrons, the whole system occurs in another intermediate state $|c_3\rangle$ with the energy

$$E_3 = W_e^{(n)} + B' + \varepsilon + \hbar\omega'. \tag{14}$$

At the last stage, the nucleus decays into a final state $|I_f M_f\rangle$, by emitting a γ quantum with the energy $\hbar\omega_\gamma$ or a conversion electron. The energy of the whole system in the final state $|b\rangle$ then becomes

$$E_b = W_f^{(n)} + B' + \varepsilon + \hbar\omega' + \hbar\omega_\gamma. \tag{15}$$

Such multistep scattering process is determined by the resonant part of the transition operator

$$\hat{T} = \hat{V}_r^{(n)} \hat{G}^+(E_a) \hat{V}_r^{(a)} \tag{16}$$

with Green's operator

$$\hat{G}^+(E_a) = (E_a + i\eta - \hat{H})^{-1}, \quad \eta \to +0. \tag{17}$$

Here, the first factor on the right-hand side of Eq. (16) describes the photoeffect induced by x-rays, and the last factor describes the emission of γ quanta by the excited nucleus.

Now, we want to present Green's operator in the form, which explicitly describes the above-discussed sequence of events (NEET followed by atomic relaxation). For this aim, we introduce the operators

$$\hat{A} = E_a + i\eta - \hat{H}, \quad \hat{B} = E_a + i\eta - \hat{H}_0 - \hat{V}_3, \tag{18}$$

where $\hat{V}_3 = \hat{V}\hat{P}_3$ and $\hat{P}_3$ are the projection operators on the vectors $|3\rangle \equiv |c_3\rangle$,

$$\hat{P}_3|b\rangle = \delta_{3,b}|b\rangle. \tag{19}$$

We use the operator identity (see also [15])

$$\hat{A}^{-1} - \hat{B}^{-1} = \hat{B}^{-1}(\hat{B} - \hat{A})\hat{A}^{-1}. \tag{20}$$

Here, the difference of $\hat{B}$ and $\hat{A}$, denoted by $\hat{V}'$, is

$$\hat{V}' = \hat{V}(1 - \hat{P}_3). \tag{21}$$

As a result, the transition operator (16) becomes

$$\hat{T} = \hat{V}_r^{(n)} \frac{1}{E_a + i\eta - \hat{H}_0 - \hat{V}_3} \hat{T}', \tag{22}$$

where the reduced transition operator

$$\hat{T}' = \hat{V}' + \hat{V}' \hat{G}^+(E_a) \hat{V}'. \tag{23}$$

The corresponding transition matrix takes the form

$$T_{ba} = \sum_{c_3, c_2, c_1} \langle b|\hat{V}_r^{(n)}|c_3\rangle \frac{1}{E_a - E_3 + i\Gamma_e^{(n)}/2} \times$$

$$\times \langle c_3|\hat{V}_r^{(a)}|c_2\rangle G_{21}^+(E_a) \langle c_1|\hat{V}_r^{(a)}|a\rangle, \tag{24}$$

where $\Gamma_e^{(n)}$ is the total width of the excited nuclear level, the summation is carried over magnetic quantum numbers and polarizations of photons.

For two overlapping resonant levels c_1 and c_2, Green's matrix $G_{c'c}^+(E_a)$ is determined by a system of algebraic equations [16]

$$(E_a - E_{c'})G_{c'c}^+(E_a) =$$
$$= \delta_{c'c} + \sum_{c''} R_{c'c''}^+(E_a)G_{c''c}^+(E_a), \qquad (25)$$

where the R matrix is represented by the expansion

$$R_{cc'}^+(E_a) = V_{c,c'} + \sum_{b \neq c,c'} \frac{V_{cb}V_{bc'}}{E_a + i\eta - E_b} + ... \qquad (26)$$

The diagonal elements of this R matrix are $R_{11} = -i\Gamma_i/2$ and $R_{22} = \Gamma_f + \Gamma_e^{(n)}$ by $R_{22} = -i(\Gamma_f + \Gamma_e^{(n)})/2$.

The solution of Eqs. (25) is given by

$$G_{11}^+(E_a) \approx \frac{1}{\Delta E - \varepsilon + i\Gamma_i/2}, \qquad (27)$$

$$G_{21}^+(E_a) \approx \frac{R_{21}}{(\Delta E - \varepsilon + i\Gamma_i/2)(\Delta E - \delta - \varepsilon + i\Gamma_f/2)}. \qquad (28)$$

Green's function $G_{21}^+(E_a)$ can be represented as a sum of two resonant terms with the poles at the points $\Delta E = \varepsilon - i\Gamma_i/2$ and $\Delta E = \delta + \varepsilon - i\Gamma_f/2$.

3. NEET Cross Section

Starting from (24), we find the cross-section of the photoinduced reaction through the NEET channel:

$$\sigma_{\text{ind}}^{(f)} = R_f \sigma_{\text{NEET}}(E), \qquad (29)$$

where the branching ratio

$$R_f = \sum_{f \neq i} \Gamma_{ef}^{(n)}/\Gamma_e^{(n)}, \qquad (30)$$

and $\Gamma_{ef}^{(n)}$ is the partial width for the nuclear transition $e \to f$.

As to the NEET cross-section, it is given by the integral over the energy $\varepsilon = \hbar^2\kappa^2/2m$ of the ejected photoelectron [13, 14]:

$$\sigma_{\text{NEET}}(E) = E_{\text{int}}^2 \left(\frac{\Gamma_f}{2\pi}\right) \times$$

$$\times \int_0^\infty \frac{\sigma_{\text{ion}}(\varepsilon)d\varepsilon}{[(\varepsilon - \Delta E)^2 + (\Gamma_i/2)^2][(\varepsilon - \Delta E + \delta)^2 + (\Gamma_f/2)^2]}. \qquad (31)$$

The cross-section $\sigma_{\text{ion}}(\varepsilon)$ is a slowly varying function of ε. Ignoring such a dependence and replacing $\sigma_{\text{ion}}(\varepsilon)$ by $\sigma_{\text{ion}} = \sigma_{\text{ion}}(0)$, one gets

$$\sigma_{\text{NEET}}(E) = P_{\text{NEET}}F_{\text{NEET}}(E)\sigma_{\text{ion}}. \qquad (32)$$

Here, the edge factor $F_{\text{NEET}}(E)$ describes the energy dependence of the NEET cross-section at the NEET edge [14]:

$$F_{\text{NEET}}(E) = \frac{1}{(1 + \Gamma_f/\Gamma_i)[\delta^2 + (\Gamma_i - \Gamma_f)^2/4]} \sum_{i=1}^3 f_i(E) \qquad (33)$$

with

$$f_1(E) = \frac{\Gamma_f}{\Gamma_i}\left[\delta^2 - \left(\frac{\Gamma_i}{2}\right)^2 + \left(\frac{\Gamma_f}{2}\right)^2\right] \times$$

$$\times \left[\frac{1}{2} + \frac{1}{\pi}\arctan\left(\frac{2\Delta E}{\Gamma_i}\right)\right], \qquad (34)$$

$$f_2(E) = \frac{\delta\Gamma_f}{2\pi}\ln\left[\frac{(\Delta E)^2 + (\Gamma_i/2)^2}{(\Delta E - \delta)^2 + (\Gamma_f/2)^2}\right],$$

$$f_3(E) = \left[\delta^2 + \left(\frac{\Gamma_i}{2}\right)^2 - \left(\frac{\Gamma_f}{2}\right)^2\right] \times$$

$$\times \left[\frac{1}{2} + \frac{1}{\pi}\arctan\left(\frac{2(\Delta E - \delta)}{\Gamma_f}\right)\right].$$

The function $F_{\text{NEET}}(E) \to 0$ at $\Delta E \to -\infty$ and $F_{\text{NEET}}(E) \to 1$ at $\Delta E \to +\infty$. The terms f_1 and f_3 correspond to two resonant terms of $G_{21}^+(E_a)$, while f_2 corresponds to their interference.

4. NEET Strength

The NEET strength E_{int}^2 equals $|R_{21}|^2$ averaged over the initial states and summed over the final states. This matrix element is determined by the second-order term of expansion (26), which describes the emission of a virtual photon by the electron and its absorption by the nucleus. If $ka \ll 1$, where $a = a_0/Z$, a_0 is the Bohr radius, and $k \approx E_0^a/\hbar c$ is the wave vector of virtual photons, one can neglect the retardation corrections to P_{NEET}, which are of the

order of 10% [11]. In such long-wave approximation, we get

$$E_{\text{int}}^2 = \frac{4\pi}{(2L+1)^2} \left(j_i L \frac{1}{2} 0 | j_f \frac{1}{2} \right)^2 e^2 \mathcal{R}_{fi}^2 \times$$

$$\times B(\lambda L; I_i \to I_e), \tag{35}$$

where j_i and j_f are the initial and final total angular momenta of the atomic shells containing the holes, which take part in NEET, and $(j_1 j_2 m_1 m_2 | jm)$ is the Clebsch–Gordan coefficient. The reduced probability of the λL transition from the initial nuclear state to the excited one is given by (see, e.g., [17])

$$B(\lambda L; I_i \to I_e) =$$
$$= \frac{1}{2I_i + 1} \sum_{\mu M_i M_e} |\langle I_e M_e | \mathcal{M}_\mu(\lambda L) | I_i M_i \rangle|^2, \tag{36}$$

where $\mathcal{M}_\mu(\lambda L)$ denotes the electric ($\lambda = E$) or magnetic ($\lambda = M$) multipole operator of the nucleus, the atomic radial matrix element

$$\mathcal{R}_{fi} = \frac{1}{a^{L+1}} \int\limits_0^\infty d\rho \rho^{-L+1} g_f(\rho) g_i(\rho) \tag{37}$$

is expressed in terms of the radial wave functions of the electron $g_{i(f)}(\rho)$ filling the $i(f)$ holes, which depend on the dimensionless radius $\rho = r/a$ and are normalized as

$$\int\limits_0^\infty g^2(\rho) \rho^2 d\rho = 1. \tag{38}$$

The nuclear electric multipole operator $\mathcal{M}_\mu(EL)$ is determined by the sum over all protons with spherical coordinates r_i, θ_i, φ_i:

$$\mathcal{M}_\mu(EL) = e \sum_{i=1}^Z r_i^L Y_{L\mu}(\theta_i \varphi_i). \tag{39}$$

Note that, in the long-wave approximation, our result (35) coincides with Harston's formula [12].

5. Absorption of X-Rays

According to the optical theorem (see, e.g., [15]), the absorption cross-section of x-rays by electrons is determined by the imaginary part of the transition matrix element T_{aa}, which is associated with the elastic scattering amplitude of x-ray photons to zero angle:

$$\sigma_{\text{a}}(E) = \frac{2}{\hbar c} \text{Im} T_{aa}. \tag{40}$$

Since the NEET matrix element $|R_{21}| \ll \Gamma_f$, the absorption of x-rays by electrons proceeds mainly without energy transfer to the nucleus. In other words, $|G_{21}^+(E_a)| \ll |G_{11}^+(E_a)|$, so that, with good accuracy,

$$T_{aa} = \sum_{m_i} \int \frac{d\boldsymbol{\kappa}}{(2\pi)^3} \langle a | \hat{V}_r^{(a)} | c_1 \rangle G_{11}^+(E_a) \langle c_1 | \hat{V}_r^{(a)} | a \rangle, \tag{41}$$

where the explicit form of G_{11}^+ is presented in (27). For the absorption cross-section of x-ray photons, we have then the following expression:

$$\sigma_{\text{a}}(E) = \frac{\Gamma_i}{2\pi} \int\limits_0^\infty \frac{\sigma_{\text{ion}}(\varepsilon) d\varepsilon}{(\varepsilon - \Delta E)^2 + (\Gamma_i/2)^2}. \tag{42}$$

Replacing again $\sigma_{\text{ion}}(\varepsilon)$ by the constant σ_{ion}, we obtain

$$\sigma_{\text{a}}(E) = F_{\text{abs}}(E) \sigma_{\text{ion}}, \tag{43}$$

where the absorption edge factor is

$$F_{\text{abs}}(E) = \frac{1}{2} + \frac{1}{\pi} \arctan \left[\frac{2\Delta E}{\Gamma_i} \right]. \tag{44}$$

6. Averaging

The cross-sections $\sigma_{\text{a}}(E)$ and $\sigma_{\text{NEET}}(E)$ should be also averaged over the energy distribution of incident photons. We approximate it by the Lorentz function:

$$w_s(E) = \frac{\Gamma_s/2\pi}{(E - \bar{E})^2 + (\Gamma_s/2)^2}. \tag{45}$$

Averaging $F_{\text{abs}}(E)$ with weight (45), we find the dependence of the averaged cross-section $\bar{\sigma}_{\text{a}}(\bar{E})$ on the mean energy of photons $\bar{E}$:

$$\mathcal{F}_{\text{abs}}(\bar{E}) = \frac{1}{2} + \frac{1}{\pi} \arctan \left[\frac{2(\Delta \bar{E})}{\Gamma_{\text{abs}}} \right], \tag{46}$$

where $\Delta \bar{E} = \bar{E} - B_i$, and the width $\Gamma_{\text{abs}} = \Gamma_s + \Gamma_i$.

By analogy, retaining only the leading term $f_3(E)$ in (33), we see that the averaged NEET cross-section $\bar{\sigma}_{\text{NEET}}(\bar{E})$ is proportional to the factor

$$\mathcal{F}_{\text{NEET}}(\bar{E}) = \frac{1}{2} + \frac{1}{\pi} \arctan \left[\frac{2(\Delta \bar{E} - \delta)}{\Gamma_{\text{NEET}}} \right], \tag{47}$$

where the width $\Gamma_{\text{NEET}} = \Gamma_s + \Gamma_M$.

It is useful to describe the K-absorption and NEET near their edges by derivatives of (46) and (47) with respect to $\bar{E}$:

$$\mathcal{F}'_{\mathrm{abs}}(\bar{E}) = \frac{(\Gamma_{\mathrm{abs}}/2)^2}{(\Delta\bar{E})^2 + (\Gamma_{\mathrm{abs}}/2)^2},$$

$$\mathcal{F}'_{\mathrm{NEET}}(\bar{E}) = \frac{(\Gamma_{\mathrm{NEET}}/2)^2}{(\Delta\bar{E} - \delta)^2 + (\Gamma_{\mathrm{NEET}}/2)^2}. \qquad (48)$$

From here, we see that Γ_{abs} and Γ_{NEET} can be interpreted as the edge widths (see also [2]).

7. NEET in Isomer $^{178}\mathrm{Hf}^{m2}$

The hafnium 16^+ isomeric level $^{178}\mathrm{Hf}^{m2}$ has the energy $W_i = 2446.09$ keV and the half-life $T_{1/2} = 31$ yr. In this state, the spin projection on the symmetry axis $K_i = 16$ much exceeds K_f of lower-lying levels. Therefore, the deexcitation transitions are strongly forbidden. This m2 isomer decays by E3 transition into the 13^- level with the energy 2433.334 keV and $K = 8$, which belongs to the rotational band with the band-head 8^- (m1 isomer), located at 1147.41 keV and having the half-life $T_{1/2} = 4$ s.

Collins *et al.* [18–24] tried to trigger the 16^+ isomer, by irradiating a target with $^{178}\mathrm{Hf}^{m2}$ by x-rays. They observed an increase of intensities for some γ-lines, as well as the appearance of new lines in the deexcitation spectrum of $^{178}\mathrm{Hf}^{m2}$, that allowed them to announce about 2% acceleration of the isomer decay. Collins *et al.* suggested that x-ray photons induced transitions into an upper-lying intermediate K-mixing level of hafnium, that cascaded up to the ground state. However, as was shown in [25–28], their results contradict the existing nuclear models. Therefore, they [19] assumed that NEET is responsible for the induced decay of the isomer. It was noted that the decay acceleration takes place at the L_3 absorption threshold [18], and the NEET probability, associated with the excitation to an intermediate nuclear state, was estimated as $P_{\mathrm{NEET}} = 1.6 \times 10^{-3}$. Such large value might be provided by E1 transitions, which are usually more intense than M1 transitions.

In the nonrelativistic approximation, we have the NEET strength at the electronic transition $M_5 \to L_3$:

$$E_{\mathrm{int}}^2 = \frac{8\pi}{9}(0.4)^{10}\left(\frac{e}{a^2}\right)^2 \times$$

$$\times \frac{(Z_i'/Z)^5(Z_f'/Z)^7}{[0.6(Z_i'/Z) + 0.4(Z_f'/Z)]^8}B(E1; I_i \to I_e), \qquad (49)$$

where Z' are effective charges due to the electronic screening of the nuclear Coulomb field. For estimations, we put $B(E1) = B_{sp}(E1)$, where the single-particle (Weisskopf) unit for the EL transition is [28]

$$B_{sp}(EL) = \frac{e^2}{4\pi}\left(\frac{3}{3+L}\right)^2 R_0^{2L}, \qquad (50)$$

and the nuclear radius $R_0 = 1.2A^{1/3}$ fm.

Estimations for the hole transition $L_3 \to M_5$ and the exact resonance ($\delta = 0$) show that the NEET probability $P_{\mathrm{NEET}} = 2.2 \times 10^{-4}$, which coincides with the result of [29]. Other types of E1 transitions appear to be much less intensive. So, for the $L_3 \to M_4$ transition, we find $P_{\mathrm{NEET}} = 3.8 \times 10^{-5}$ compared to 4.4×10^{-5} of [29] and 2.8×10^{-5} of [30]. For the $L_3 \to M_1$ transition, $P_{\mathrm{NEET}} = 2.1 \times 10^{-6}$, whereas $P_{\mathrm{NEET}} = 3.8 \times 10^{-6}$ in [29] and 8.0×10^{-6} in [30].

Since the experimental shift of the NEET peak $\Delta E = 6$ eV [18], we ought to put $\delta = 3.5$ eV. Then the corrected NEET probability for the $M_5 \to L_3$ electron transition becomes $P_{\mathrm{NEET}} = 0.9 \times 10^{-4}$. The edge factor $F_{\mathrm{NEET}}(E) = 1$ at all energies of x-ray photons $\Delta E \gg \delta + \Gamma_f$. This means that the accelerated decay of the hafnium isomer had to be observed at all energies above the NEET threshold. Therefore, it is strange that the decay acceleration have been detected [18] only in a narrow interval of the order of 1 eV above the L_3 edge.

8. Intermediate Triaxial Shape

The probability P_{NEET} of the photoinduced NEET for isomer $^{178}\mathrm{Hf}^{m2}$ has been calculated with the use of quantum electrodynamics in [29, 30]. It was believed that $^{178}\mathrm{Hf}$ in the hypothetical intermediate state 15^- conserves the prolate axial shape. In this case, its spin projection on the symmetry axis has the definite value $K_e = 15$. As a result, the transitions $15^- \to 13^-$ with the alteration of K by $\Delta K = 7$ should be strongly forbidden as compared with the backward transition $15^- \to 16^+$ with $\Delta K = 1$. The corresponding extremely small branching ratio $R \sim 10^{-14}$ [29, 30] absolutely annihilates the results of Collins *et al.* But one cannot exclude the situation where the nucleus in an intermediate state attributes a triaxial shape. Then the wave function $|I_e M_e\rangle$ will be spread over the states with different K_e [17]:

$$|I_e M_e\rangle = \sum_{K_e}\sum_{\Omega_e} A^{I_e \tau}_{K_e, \Omega_e}(\gamma)|I_e M_e K_e \Omega_e\rangle. \qquad (51)$$

Here, the basis components $|I_e M_e K_e \Omega_e\rangle$ are given by

$$|I_e M_e K_e \Omega_e\rangle = \sqrt{\frac{2I_e + 1}{16\pi^2}} \times$$

$$\times \left[D^{I_e}_{M_e K_e}(\vartheta)\chi_{\Omega_e}(\mathbf{r}') + (-1)^{I_e} D^{I_e}_{M_e,-K_e}(\vartheta)\chi_{-\Omega_e}(\mathbf{r}') \right], \tag{52}$$

where $D^{I_e}_{M_e K_e}(\vartheta)$ is the rotation matrix depending on the Eulerian angles $\vartheta = \{\vartheta_1, \vartheta_2, \vartheta_3\}$, which determine the orientation of the coordinate frame ξ, η, ζ bound to the principal axes of the inertia ellipsoid of the nucleus, K_e and Ω_e are the projections of the total ($\mathbf{I}$) and intrinsic ($\mathbf{j}$) angular momenta on the axis ζ, and the function $\chi_{\Omega_e}(\mathbf{r}')$ describes the intrinsic motion of nucleons with coordinates $\mathbf{r}'$ relative to the axes ξ, η, ζ. The projections take the values $K_e = 1, 3, \ldots, 15$ and $\Omega_e = 1, 3, \ldots$.

The expansion coefficients $A^{I_e \tau}_{K_e, \Omega_e}(\gamma)$, depending on the triaxiality parameter γ, satisfy the following orthogonality relations:

$$\sum_{K_e \Omega_e} A^{I_e \tau}_{K_e, \Omega_e}(\gamma) A^{I_e \tau'}_{K_e, \Omega_e}(\gamma) = \delta_{\tau \tau'},$$

$$\sum_{\tau} A^{I_e \tau}_{K_e, \Omega_e}(\gamma) A^{I_e \tau}_{K'_e, \Omega'_e}(\gamma) = \delta_{K_e K'_e} \delta_{\Omega_e \Omega'_e}. \tag{53}$$

The equations to determine the coefficients $A^{I_e \tau}_{K_e, \Omega_e}(\gamma)$ in odd triaxial nuclei can be found in [17].

A similar K-mixing arises if the nucleus in the 15^- state is γ-soft. Then it can be treated as a rigid triaxial rotator with the effective triaxiality parameter γ_{eff} [17]. We recall that the maximum mixing of components with different K_e is achieved when $\gamma_{\text{eff}} = \pi/6$. The initial isomeric state 16^+ with the prolate axially symmetric shape ($\gamma = 0$) is described by the single component $|16, M_i, 16, 16\rangle$.

When we pass to the axes ξ, η, ζ, the electric multipole operator (37) transforms as

$$\mathcal{M}_\mu(EL) = \sum_\nu D^L_{\mu\nu}(\vartheta) \mathcal{M}'_\nu(EL), \tag{54}$$

where $\mathcal{M}'_\nu(EL)$ depends on the intrinsic coordinates $\mathbf{r}'_i$. By using also the integral

$$\int D^{I_f}_{M_f K_f}(\vartheta)^* D^L_{\mu\nu}(\vartheta) D^{I_e}_{M_e K_e}(\vartheta) d\Omega =$$

$$= \frac{8\pi^2}{2I_f + 1}(I_e L M_e \mu | I_f M_f)(I_e L K_e \nu | I_f K_f), \tag{55}$$

we find the reduced probability for the EL transition per unit time from the excited state $I_e = 15^-$ to any final axially symmetric state $|I_f M_f K_f, \Omega_f\rangle$ with $\Omega_f = K_f$:

$$B(EL; I_e \to I_f) = \left| \sum_\nu \sum_{K_e, \Omega_e} A^{I_e}_{K_e, \Omega_e}(\gamma) \times \right.$$

$$\left. \times (I_e L K_e \nu | I_f K_f)\langle \chi'_{K_f} | \mathcal{M}'_\nu(EL) | \chi_{\Omega_e}\rangle \right|^2. \tag{56}$$

Every intrinsic wave function $\chi_\Omega(\mathbf{r}')$ can be expanded in the functions $|j\Omega\rangle$ characterized by a definite angular momenta j:

$$\chi_\Omega(\mathbf{r}') = \sum_j a_j |j\Omega\rangle. \tag{57}$$

Then

$$\langle \chi'_{\Omega_f} | \mathcal{M}'_\nu(EL) | \chi_{\Omega_e}\rangle =$$

$$= \sum_{j_f j_e} a^*_{j_f} a_{j_e}(j_e L \Omega_e \nu | j_f \Omega_f)\langle j_f || \mathcal{M}'(EL) || j_e\rangle|^2, \tag{58}$$

where $\Omega_f = K_f$, and $\langle j_f || \mathcal{M}'(EL) || j_e\rangle$ denotes the reduced matrix element. From Eqs. (56) and (58), it follows that $K_f = K_e + \nu$ and $K_f = \Omega_e + \nu$. In other words, only the components with $K_e = \Omega_e$ of the 15^- wave function are involved in the electromagnetic transition.

To estimate $B(EL)$, we demand that, for every transition,

$$|\langle \chi'_{\Omega_f} | \mathcal{M}'_\nu(EL) | \chi_{\Omega_e}\rangle|^2 = B_{sp}(EL). \tag{59}$$

Then, in correspondence with (56) for the E1 transition from 15^- to 16^+, we have

$$B(E1; 15^- \to 16^+) = \left(A^{15}_{15,15}(\gamma) \right)^2 B_{sp}(E1), \tag{60}$$

while, for the E2 transition from $I_e = 15^-$ to $I_f = 13^-$ with the energy 2433.334 keV and the spin projection $K_f = 8$,

$$B(E2; 15^- \to 13^-) \sim$$

$$\sim \left| \sum_{K_e, \nu} A^{15}_{K_e, K_e}(\gamma)(15, 2, K_e \nu | 13, 8) \right|^2 B_{sp}(E2), \tag{61}$$

where $K_e = 6, 8, 10$.

The unit-time probability for the EL transition is related to the reduced probability by [17]

$$P(EL; i \to f) = \frac{8\pi(L+1)}{\hbar L[(2L+1)!!]^2} k^{2L+1} \times$$

$$\times B(EL; i \to f), \tag{62}$$

where k is the wave vector of emitted γ-quanta.

Substituting (60) and (61) in (62) and adopting that all the expansion coefficients $A_{K_e, K_e}^{15}(\gamma)$ are approximately equal, we arrive at the branching ratio

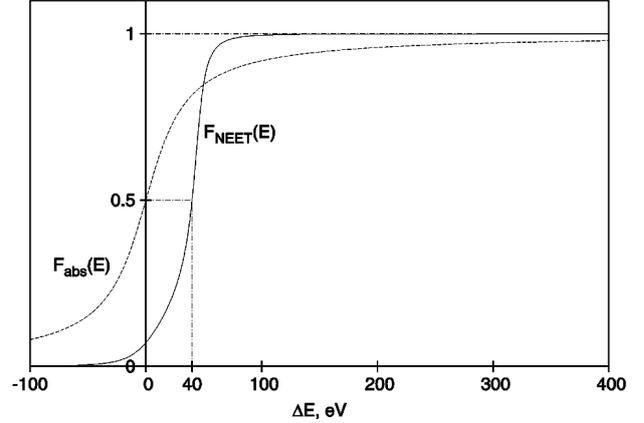$$R = \frac{P(E2; 15^- \to 13^-)}{P(E1; 15^- \to 16^+)} \sim 10^{-7}, \tag{63}$$

but not at $R \sim 10^{-14}$, as predicted in [29, 30].

9. Discussion

The behavior of the NEET and K-absorption cross-sections for ^{197}Au in a vicinity of the K-absorption threshold is shown in the figure. We found that the NEET edge defined by $F(E_*) = 0.5$ is located at $\delta = 40$ eV if the energy shift $\Delta E_* = 45$ eV. This value lies between two experimental values, discussed in Introduction. The exact equality of δ and ΔE_* is achieved only when we take the leading term $f_3(E)$ of the edge factor $F(E)$ into account. Perhaps, the analysis of slight oscillations of the NEET curve observed by Kishimoto *et al.* [2] might lead to a better agreement with one of the experimental data. Our approach allows one to understand why the NEET events for ^{197}Au appear in a vicinity of the K-absorption threshold $\Delta E = 0$ and rapidly grow at another resonant point $\Delta E \approx \delta$. For this aim, we rewrite the energy conservation law $E_b = E_a$ as

$$\varepsilon = \Delta E - \delta - \hbar(\omega' - \omega_0'). \tag{64}$$

Here, we took into account that the energy of a γ-quantum emitted by the nucleus practically coincides with the transition energy. The photoemission of K-electrons appears even at $\Delta E \approx 0$ owing to the large width Γ_{M_1} of the M_1-hole. In other words, the NEET channel becomes open ($\varepsilon > 0$) when x-ray photons, emitted during the filling of the M_1-hole, have the energy $\hbar\omega' \sim \hbar\omega_0' - \delta$ that corresponds to the emission line wing. Therefore, the NEET process, being weak at $\Delta E \approx 0$, sharply grows only at $\Delta E \approx \delta$ in correspondence with [2].

NEET edge function $F_{\text{NEET}}(E)$ (solid) and K-absorption factor $F_{\text{abs}}(E)$ (dashed), calculated for nucleus ^{197}Au, versus the energy E of x-ray photons, where $\Delta E = E - B_K$, and B_K denotes the binding energy of the K-electron

The width of the NEET edge Γ_{NEET} is much less than that of the K-absorption edge Γ_{abs}, because $\Gamma_K \gg \Gamma_M$. For ^{197}Au by means of Eqs.(48), we found $\Gamma_{\text{NEET}} = 17.8$ eV and $\Gamma_{\text{abs}} = 55.5$ eV, which well correlates with the experimental data $\Gamma_{\text{NEET}} = 14 \pm 9$ eV, $\Gamma_{\text{abs}} = 58 \pm 3$ eV [2].

We also analyzed the NEET mechanism as a possible explanation of the intriguing experiments of Collins *et al.* The hafnium atomic binding energies are $B(L_3) = 9560.7 \pm 0.4$ eV and $B(M_5) = 2600.9 \pm 0.4$ eV [33], so that the electron transition energy $E_0^a = 6.9598$ keV. The energy of the nuclear transition, involved in NEET, differs from E_0^a only by a few eV [18]. Therefore, the intermediate level 15^- should have the energy $W_e = 2453.05$ keV.

Note that our nonrelativistic calculations of the probability P_{NEET} for the excitation of the intermediate 15^- level via atomic electrons correlate with more exact relativistic Hartree–Fock calculations [29, 30]. Therefore, analyzing NEET in other nuclei, one can apply analogous simple estimations. Above the L_3 absorption edge, we found $P_{\text{NEET}} = 0.6 \times 10^{-4}$, being less than the experimental value $P_{\text{NEET}} \times R = 1.6 \times 10^{-3}$ [18].

Up to now, the main theoretical argument against the validity of the experimental results [18] was a very low branching ratio R for the deexcitation transition of the 15^- level into the 13^- level against the transition, which returns the nucleus back in the 16^+ isomeric state [29, 30].

The assumption of the triaxiality of the nuclear shape in the 15^- state allows us to increase the previous estimations of R by 7 orders. However, our estimation (63) again shows that the deexcitation path $15^- \to 13^-$ is too weak to be possible. The main reason is that the 13^- level is separated only by 19.72 keV from the 15^- level. The situation is improved if there is one more 13_1^- level, which is situated much lower. Let the energy of transition $15^- \to 13_1^-$ be 400 keV. Then we already get $R \sim 1$. Note, however, that the expansion amplitude $A_{15,15}^{15}$ is greater than all other amplitudes A_{K_e,Ω_e}^{15} with $K_e, \Omega_e < 15$, and, hence, the above value of R can be overestimated. Of course, our estimations are very rough, and a more fundamental theory of electromagnetic transitions in triaxial nuclei similar to that given in [17] for odd nuclei, which were treated as an even-even core + one nucleon, is needed.

Since the m2 isomer spontaneously decays to the 13^- level, but not in any hypothetical $f = 13_1^-$ level, we ought to assume also that the corresponding spin projection $K_f < 8$, where $K = 8$ characterizes the 13^- state. This is possible if the 13_1^- level belongs to any yet unknown rotational band with $K_f < 8$. Then the decay will occur around the rotational band built on the m1 isomer. Such our conclusion correlates, in principle, with the statement of [18]. In this experiment, an induced prompt decay of the isomer has been detected around the 13^- level. On the contrary, the decay to the 13^- level (member of the rotational band of the m1 isomer) would lead to a 4-s delay of the emission of γ quanta.

Thus, if nucleus ^{178}Hf has a triaxial shape in the intermediate state 15^-, it can successfully decay to the 13_1^- level of a still unknown rotational band. However, even in such favorite case, our upper estimation of the effect remains less than the experimental data by one order. The possible collectivity of the 15^- level would increase the NEET probability.

At the same time, the decay should be observed at all energies E of x-ray photons above the L_3 absorption threshold (see the figure), whereas, in the experiment [18], the decay enhancement vs E has been described by a very sharp peak. Perhaps, such a peak appeared since experimentalists concentrated only on the narrow range of x-ray energies above the L_3 absorption edge.

Although the alternative experiments with synchrotron radiation [31, 32] did not confirm the results of Collins's team [1–6], we see no basic objections against their findings, and the question about the induced depletion of ^{178}Hf^{m2} remains challenging.

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ЗБУДЖЕННЯ ЯДЕР
ЕЛЕКТРОННИМ ПЕРЕХОДОМ

Р е з ю м е

На основі строгої теорії зіткнень розвинуто теорію збудження ядер електронним переходом (NEET), індукованим рентгенівськими променями. Розглянуто всі стадії процесу, включаючи утворення вакансії у внутрішній електронній оболонці, її розпад, що приводить до збудження ядра, та подальше заповнення вакансії на вищому рівні разом із розрядкою ядра. Розраховано перерізи для NEET та фотопоглинання рентгенівських променів поблизу краю поглинання. Результати узгоджуються з даними Кішімото та інших для NEET на ^{197}Au. Крім того, ми обговорюємо NEET, як механізм тригерування 31-річного ізомеру ^{178}Hf^{m2} через проміжний рівень. Показано, що 2% прискорення розпаду цього ізомеру, яке спостерігалося Коллінсом та ін., реально, якщо ядро набуває в проміжному стані неаксіальної форми та існує ще додаткова обертальна смуга з рівнем 13^-.