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**CONVERSION PROBABILITIES
OF LOW-ENERGY ($\hbar\omega \leq 3$ keV) NUCLEAR TRANSITIONS
IN THE ELECTRON SHELLS OF FREE ATOMS**

**D.P. Grechukhin
and
A.A. Soldatov**

**Article Translated from Journal Yadernye Konstanty
(Nuclear Constants)**

Series: Nuclear Constants, Issue No. 1, 1987

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June 2005

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Abstract

CONVERSION OF LOW-ENERGY NUCLEAR TRANSITIONS ($\hbar\omega \leq 3$ keV) IN THE OUTER ELECTRON SHELLS OF AN ISOLATED ATOM. Conversion of some low-energy transitions ($\hbar\omega \leq 3$ keV) in the nuclei ^{90}Nb , ^{99}Tc , ^{103}Ru , ^{110}Ag , ^{140}Pr , ^{142}Pr , ^{153}Gd , ^{159}Gd , ^{160}Tb , ^{165}Tm , ^{171}Lu , ^{173}W , ^{188}Re , ^{193}Pt , ^{204}Hg , ^{205}Pb , ^{236}Pa and ^{250}Bk are investigated for the case of an isolated atom. The conversion transition probabilities are calculated using the electron wave functions, obtained through numerical integration of the Dirac equations in the atomic field within the framework of the Hartree-Fock-Slater method. The calculation is carried out for the normal configuration of the valence band of the aforementioned atoms. The calculation results are tabulated in this paper.

* Tables of the electronic factors of the conversion probabilities may be obtained in full from the Centre for Nuclear Structure and Reaction Data (CAJAD) of the USSR State Committee on the Utilization of Atomic Energy from the following address: I.V. Kurchatov Institute of Atomic Energy, Centre for Nuclear Structure and Reaction Data, 123182 D-182, Moscow.

Here, the authors have limited themselves to instructions for their use based on the example of the nucleus $^{90}\text{Nb}_{41}$.

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Introduction

1. In the case of low-energy nuclear transitions $E_1I_1 \rightarrow E_2I_2$, ($\hbar\omega = E_1 - E_2 \lesssim 3$ keV; I_1I_2 is the spin of the nucleus in the initial and final states), the electrons in the atomic shell are actually in the static region of the nuclear ΛL multipole (ML or EL); the case of E0 conversion is not considered. The probability of internal conversion in such transitions is substantially greater than the probability of gamma-ray photon emission by the nucleus. In this situation, it is more natural to operate directly with the conversion probability than with the internal conversion coefficients (ICCs), which have extremely large values here and attain values which are in fact unobservable. Experimental ICCs are essentially determined by photon re-emission along the 'electron bridge' channel: first the nuclear transition ejects an electron from the atomic shell and then that electron 'sits' in the hole formed by the gamma-ray photon emission. The valence band electrons [orbital binding energy $\varepsilon \leq \frac{1}{2} (e^2/a_0) = 13.6$ eV] and the outer filled shell electrons [$\varepsilon \leq (2-3) e^2/a_0$] participate actively in the conversion process at the energies under investigation. The structure of the outer electron orbits is determined by the type of environment of the atom under study in the molecule or the condensed medium into which the atom labelled by the isomeric nucleus has been introduced. The variations in the decay rate constant λ (or the isomer lifetime τ) caused by a change in the chemical environment of the initial nuclear state are sufficiently large and accessible for experimental research. A summary of the data accumulated up to 1972 on variations in the λ constants for certain isotopes, including for conversion transitions in the nuclei ^{90}Nb , ^{99}Tc , ^{193}Pt and ^{235}U , is given in the review contained in Ref. [1]. For conversion isomers, the current experimental status is given in the review contained in Ref. [2].

The change in the decay rate constant λ has been studied in particular detail for E3 transitions of the isomers $^{235\text{m}}\text{U}$ ($\hbar\omega = 76.8 \pm 0.5$ eV) [3–5], $^{99\text{m}}\text{Tc}$ [6] and $^{90\text{m}}\text{Nb}$ (mixed E3+M2 transition) [7]. In the case of introducing the uranium and niobium isomers into metals [4, 5, 7], changes $\delta\lambda/\lambda \approx 3\text{--}5\%$ have been discovered. These changes in the conversion transition rate constant of the nucleus during introduction into a medium or the formation of a chemical compound are caused by various mechanisms; the manifestation of these reflects the characteristics of the conversion process. The effects are particularly clearly pronounced during low energy transitions ($\hbar\omega$ of a few kilo-electron-volts). A general investigation of the conversion process in relation to the effects of the atom's chemical environment is given in Ref. [8].

In the region of low-energy nuclear transitions, when the quantum wavelength $\lambda = c/\omega$ is greater than the size of the atomic shell, the electromagnetic potentials of the ΛL multipolarity transition have a dependence in the form of $(1/r)^{L+1}$ on the distance r from the nucleus of the isomer, i.e. the conversion takes place in the static multipole field region. As a result, the radial integrals of the interaction of the electron with the transition field of the nucleus, which determine the conversion probabilities, accumulate at short distances in the region of the radius $R \approx 0.1 a_0$ ($a_0 = \hbar^2/me^2 = 5.2917 \cdot 10^{-9}$ cm — the Bohr radius) for the M1, E2, M2, E3 and higher multipoles (exception for E1). This fact was initially emphasized by Slater [9], a general qualitative investigation of the character of the spatial formation of ICCs has been made by Sliv et al. [10], and more specific qualitative characteristics for some of the

conversion isomers studied have been obtained by the authors of Refs [8, 11].

In the conversion region, the shape of the electron wave functions is mainly determined by the strong Coulomb field of the nucleus and so functions with the same orbital (ℓ) and angular (j) momenta have a weak energy dependence. This dependence is shown in the amplitude of the electron wave function in the vicinity of the nucleus [8]. When the atom is introduced into a medium or during formation of the molecule, the orbits of the converging electrons are distorted. Here, there is a possibility of both the numerical values of the amplitudes of radial components of the wave function in the vicinity of the isomeric nucleus (squeezing-stretching of the orbit) and hybridization of the orbits caused by the spatial structure of the perturbation field of neighbouring atoms. These effects are reflected in redistribution of the amplitudes of the expansion of wave functions with respect to states with momenta (ℓj). Both effects (squeezing-stretching and hybridization) can be observed for both coupled orbits and continuous electron spectrum states. The effects should decrease exponentially as the orbital binding energy increases. For the outermost coupled orbits, the scale of the changes induced during strong orbit deformation can be evaluated if these effects are imitated by changing the population density of the atomic orbits, i.e. by varying the valence band configuration structure of the atomic shell. Just such a simplified evaluation of the possible scale of $\delta\lambda$ has been carried out for the E3-isomer of ^{235m}U using an exhaustive method of possible configurations of the six outer electrons of the atomic shell [12]. We established the presence of a strong modifying effect of the number of $5f$ electrons on the conversion probability from filled $6p$ orbits [$\delta\lambda/\lambda \approx 8\%$ when $\Delta N(5f)=1$], although $5f$ electrons themselves make a negligible direct contribution to the E3-isomer conversion probability.

Along with change in the states of the electrons belonging to a fixed atom, during atom interaction there is leaking (delocalization) of electrons previously belonging to isolated neighbouring atoms in the vicinity of the isomeric nucleus. This delocalization effect opens a new conversion channel that is absent in the isolated atom situation, which also produces a change in $\delta\lambda$. Apart from the orbit hybridization effects, this conversion channel is of particular interest in researching the electron shell structure.

2. The classification of effects given is of course provisional, but it provides a qualitative indication of the structure of possible types of electron orbit deformation resulting in a change in the $\delta\lambda$ constants in conversion transition of the nucleus. It is clear that the values of $\delta\lambda$ observed experimentally are cumulative both with respect to the contributions of the different electron orbits included in the conversion process and the aforementioned types of deformation that these orbits undergo during atom interaction. The values of $\delta\lambda/\lambda$ themselves are, as a rule, not informative; of course higher values point to significant rearrangement of the electron shell, but a small value does not necessarily mean that the shell has not changed much because the contribution of various orbits to $\delta\lambda$ may have different signs. Considerably more detailed information on the structure of the electron shell is contained in the differential spectrum of the conversion electrons that is split into individual lines (or groups of close lines) corresponding to conversion from separate electron orbits. For the isomers ^{235m}U and ^{99m}Tc , such spectra with an energy resolution of approximately 1 eV have already been studied in Refs [13, 14]. The variations in the partial conversion probabilities of the ΛL nuclear transition in separate electron orbits should be considered as a key subject of experimental and theoretical research. In order to be able to evaluate the nature and extent of rearrangement of the electron shell during atom interaction from the conversion electron spectra, reference data is required on the partial conversion probabilities for the case when the atom is in fixed 'standard' conditions. This of course does not obviate the need for subsequent calculation of the conversion spectrum for each specific chemical compound or cluster. A

similar kind of extremely time-consuming calculation may be undertaken with respect to the electron orbit wave functions, identified for example using the X- α scattered wave method by means of numerical integration of the Dirac equation in the self-consistent multicentre field of a molecule or cluster. This method of analysis is already being successfully used with respect to technetium compounds [14]; for the isomer ^{235m}U , it is necessary to establish the functions of the continuous electron spectrum in the cluster field.

The situation of an isolated free atom constitutes a form of reference conditions for existence common to all atoms. In this situation the conversion spectrum can be calculated using different variants of the Hartree-Fock method. Unfortunately, this ideal situation almost never occurs in experimental conditions; the atoms in the targets always have neighbouring atoms which have a considerable influence on the state of electrons with binding energies up to approximately $2e^2/a_0$ (approximately 60 eV) [13, 14]. Nevertheless, detailed calculations of the partial conversion probabilities of ΛL multipoles in the electron shell of an isolated atom are necessary above all for preliminary analysis of experimental spectra in order to determine the region of the spectrum with the greatest deviation from the reference spectrum, since for deep orbits there can be a correlation with the reference spectrum. These data are also needed for a rough initial evaluation of the possible amplitude of the $\delta\lambda/\lambda$ variations during changes in the configuration of the valence band. Furthermore, the reference conversion probabilities obtained allow the values of the nuclear matrix elements carrying information on the structure of the nuclear states to be found from the known half-lives of the conversion isomer. We shall comment on two isomers: ^{235m}U and ^{90m}Nb . In the case of the isomer ^{235m}U , an E3 transition matrix element has been found [11], which was close in magnitude to a proton single-particle element, although in the case of the $^{235}\text{U}_{92}$ nucleus a change occurs in the odd neutron state. This high intensification of the E3 transition, it has turned out, is attributable to excitation of the octupole vibrations of the shell (of the ^{234}U nucleus). The similar calculation we performed for the conversion probabilities of the isomer ^{90m}Nb showed an extremely pronounced deceleration of the M2 transition, caused by mutual cancellation of the M2 transition contributions of the proton and neutron holes $(1f5/2)^{-1} \rightarrow (1g9/2)^{-1}$ in the shell of the $^{90}\text{Nb}_{41}$ nucleus.

Bearing in mind the application areas given above for the partial conversion probabilities, the authors will include in this paper the calculation results of the conversion coefficients for nuclear ΛL transitions with energies $\hbar\omega \lesssim 3$ keV for a group of selected isotopes. Unlike the standard ICC tables, for each nucleus we examined the conversion process for a transition with a fixed multipolarity in an energy interval limited by experimental measurement error. A relativist variant of the Hartree-Fock-Slater method (as amended by Latter) [HFS(L)] was used to calculate the central field of the atom and the electron wave functions [15, 16].

Conversion probabilities of a ΛL nuclear transition in the $(n\ell j)$ -orbit of an isolated atom.

1. Let us consider the ΛL multipolar transition of a nucleus with energy $\hbar\omega = E_1 - E_2$ from the state $| E_1 I_1 M_1 \rangle$ to the final state $| E_2 I_2 M_2 \rangle$, where $E_i I_i M_i$ are the energy, spin and spin projection of the nucleus in the i th state, respectively. In this process an electron from the shell of the atom in the state $| \varepsilon_1 n_1 \ell_1 j_1 \mu_1 \rangle$ with energy ε_1 (primary quantum number n_1 , orbital momentum ℓ_1 , angular momentum j_1 (μ_1 — magnetic projection of the vector j_1)) will transit into the continuous spectrum state with energy $\varepsilon = \hbar\omega + \varepsilon_1$. Hereinafter, the full (relativistic) energy of the electron $\varepsilon = [(mc^2)^2 + \hbar^2 c^2 p^2]^{1/2}$ is always used, since the conversion process takes place at small distances from the nucleus and, consequently, the wave functions of the electron in an initial state $| \varepsilon_1 n_1 \ell_1 j_1 \mu_1 \rangle$ and a final state $| \varepsilon p \rangle$ are necessarily relativistic, despite

the fact that at nuclear transition energies $\hbar\omega \leq 3$ keV (which are considered here) only loosely bound electron orbits in the shell of the atom are affected by the conversion process.

The theory of the conversion of nuclear ΛL multipoles in electron orbits has long been a ‘classic’ chapter in quantum electrodynamics and has been examined in great detail in the available literature (see, for example, Refs [17, 18]). Thus, without lingering on the calculation details, we will give the resulting formula for the conversion probability in a unit of time for a nuclear ΛL multipole in EL and ML transitions ($L \neq 0$), based on one electron of an $(n_1 \ell_1 j_1)$ -orbit population in the atomic shell. This is indicated below by $[n_1 \ell_1 j_1]^1$. Averaging and summation, respectively, are carried out with respect to the unobservable quantum numbers of the initial and final states:

$$W(\Lambda L; I_1 \rightarrow I_2; \varepsilon_1 [n_1 \ell_1 j_1]^1 \rightarrow \varepsilon) = e^4 m / \hbar^3 (R_0 a_0)^{2L} w_e(\Lambda L [n_1 \ell_1 j_1]^1 \hbar\omega) \langle I_2 \| \Lambda L \| I_1 \rangle^2, \quad (1)$$

where $\varepsilon = \varepsilon_1 + \hbar\omega$; $e^4 m \hbar^{-3} = 4.1341 \cdot 10^{16} \text{ c}^{-1}$; $\varepsilon_1 \lesssim mc^2$; $a_0 = \hbar^2 / me^2 = 5.2917 \cdot 10^{-9}$; R_0 is the nuclear radius.

If there are $N(n_1 \ell_1 j_1)$ electrons in the electron orbit $(n_1 \ell_1 j_1)$, then the full conversion probability from this orbit is equal to the product:

$$N(n_1 \ell_1 j_1) W(\Lambda L; I_1 \rightarrow I_2; \varepsilon_1 [n_1 \ell_1 j_1]^1 \rightarrow \varepsilon). \quad (2)$$

Here, it is expedient to introduce the partial conversion coefficient of the $(n_1 \ell_1 j_1)$ orbit, in accordance with the formula:

$$\xi(n_1 \ell_1 j_1; \Lambda L) = N(n_1 \ell_1 j_1) w_e(\Lambda L [n_1 \ell_1 j_1]^1 \hbar\omega) \quad (3)$$

This coefficient fixes the structure of the observable electron conversion spectrum. Below, only the case $L \neq 0$ is considered, and so the general scale coefficient $(R_0 a_0)^{2L}$ is assigned in the probability formula; the value $R_0 = 1.24 \cdot 10^{-13} \text{ A}^{1/2} \text{ cm}$ is taken for the nuclear radius in the calculations.

The wave functions of the initial and final electron states were arrived at by taking into account the final dimensions of the nucleus, whose Coulomb field was approximated using the field of a uniformly volume-charged sphere with a radius of R_0 . The dimensionless reduced nuclear elements $\langle I_2 \| \Lambda L \| I_1 \rangle$ were determined by the equations:

$$\begin{aligned} eR_0^L \langle I_2 \| EL \| I_1 \rangle C_{LM_1 M_1}^{I_2 M_2} = \\ = \langle E_2 I_2 M_2 \left| \int (d\vec{r}) r^L Y_{LM}(\vec{r}) \hat{\rho}_N(\vec{r}) \right| E_1 I_1 M_1 \rangle \end{aligned} \quad (4)$$

(where $\hat{\rho}_N(\vec{r})$ is the nuclear charge density operator);

$$\begin{aligned} eR_0^L \langle I_2 \| ML \| I_1 \rangle C_{LM_1 M_1}^{I_2 M_2} = \\ = \langle E_2 I_2 M_2 \left| \frac{1}{c} \int (d\vec{r}) r^L \left[\vec{Y}_{LLM}(\vec{r}) \hat{j}_N(\vec{r}) \right] \right| E_1 I_1 M_1 \rangle \end{aligned} \quad (5)$$

(where the charge current density operator $\hat{\vec{j}}_N(\vec{r})$ is linked to the charge density operator by means of the conservation correlation:

$$\text{div} \hat{\vec{j}}_N + \frac{\partial \hat{\rho}_N}{\partial t} = 0). \quad (6)$$

Here, the spherical vector harmonics $\vec{Y}_{LLM}(\vec{r})$ determined in [7] and the Clebsch-Gordan coefficients $C_{LM_1 M_2}^{I_2 M_2}$ are used.

The dimensionless reduced nuclear matrix elements $\langle I_2 \parallel \Lambda L \parallel I_1 \rangle$ ($L \neq 0$) are linked with the reduced probabilities $B(\Lambda L; I_1 \rightarrow I_2)$ of a nuclear ΛL multiplet $I_1 \rightarrow I_2$ transition taken in Refs [19, 20] by means of the correlations:

$$e^2 R_0^{2L} \frac{2I_2 + 1}{2I_1 + 1} |\langle I_2 \parallel \text{EL} \parallel I_1 \rangle|^2 = B(\text{EL}; I_1 \rightarrow I_2); \quad (7)$$

$$e^2 R_0^{2L} \frac{L}{L+1} \frac{2I_2 + 1}{2I_1 + 1} |\langle I_2 \parallel \text{ML} \parallel I_1 \rangle|^2 = B(\text{ML}; I_1 \rightarrow I_2). \quad (8)$$

The apparently disparate notation in formulas (1) and (2) for the EL and ML multipoles was caused by the original choice of determination of the electron coefficient $w_e(\Lambda L [n\ell j]^1 \hbar\omega)$, which was then numerically tabulated specifically in those terms. Redetermining that coefficient by including the $L/L+1$ multiplier was thought unnecessary by the authors.

2. The single electron conversion coefficients of the nuclear ΛL -multipoles ($L \neq 0$) may be expressed in the form:

$$w_e(\Lambda L [n_1 \ell_1 j_1]^1 \hbar\omega) = 32\pi^2 \frac{(ka_0)^{2L+2}}{[(2L+1)!!]^2} \frac{1}{(pa_0)} \frac{\varepsilon + mc^2}{mc^2} \times \quad (9)$$

$$\times 1/(2L+1)(2j_1+1) \sum_{(j\ell)} (2j+1) |A(j\ell; \Lambda L; j_1 \ell_1)|^2 |\langle j\ell [\Lambda L \ell] j_1 \ell_1 \rangle|^2,$$

where p is the wave number of the escaping electron; $k = \omega/c$; $\varepsilon = [m^2 c^4 + \hbar^2 c^2 p^2]^{1/2}$. Here, a system of radial integrals $\langle j\ell \mid [\Lambda L \ell] \mid j_1 \ell_1 \rangle$ was introduced; when calculating these, the relativistic wave functions of the initial and final states of the electrons, with the fixed angular momenta $(j_1 \ell_1)$ and $(j\ell)$, respectively, were used. The functions were obtained through numerical integration of the Dirac equations with the central atomic field of the Hartree-Fock-Slater model [16]:

$$\begin{aligned}
\langle j\ell[\text{ELel}]|j_1\ell_1\rangle &= \int_0^\infty dx h_L^{(1)}(ka_0x)(G_{\ell_j}g_{\ell_1j_1} + F_{\ell_j}f_{\ell_1j_1}) - \\
&- \int_0^\infty dx h_{L-1}^{(1)}(ka_0x)(F_{\ell_j}g_{\ell_1j_1} - G_{\ell_j}f_{\ell_1j_1}) + \frac{1}{L}[(j+1)j - \\
&- (j_1+1)j_1 + (\ell_1+1)\ell_1 - (\ell+1)\ell] \int_0^\infty dx h_{L-1}^{(1)}(ka_0x)(F_{\ell_j}g_{\ell_1j_1} + G_{\ell_j}f_{\ell_1j_1}).
\end{aligned} \tag{10}$$

For the ML multipole, we have:

$$\langle j\ell[\text{ML el}]|j_1\ell_1\rangle = \int_0^\infty dx h_L^{(1)}(ka_0x)(G_{\ell_j}f_{\ell_1j_1} + F_{\ell_1}g_{\ell_1j_1}). \tag{11}$$

In expressions (3) and (4), $h_N^{(1)}(z)$ is a spherical Hankel function of the first kind. The radial components (large G_{ℓ_j} and small F_{ℓ_j}) of the continuous electron spectrum states are normalized in such a way that in the asymptotics, the large components have the form:

$$G_{\ell_j}(r)|_{r \rightarrow \infty} \rightarrow \sin\left(pr - \frac{\ell\pi}{2} + \delta_{\ell_j}\right). \tag{12}$$

For the bound states, we have the standard:

$$\int_0^\infty dx (g_{\ell_1j_1}^2 + f_{\ell_1j_1}^2) = 1. \tag{13}$$

The angular integrals from the electron spherical spinors $\Omega_{j\ell m}$ [17] are introduced in accordance with the determination for the electric multipole EL:

$$A(j\ell; \text{EL}; j_1\ell_1) C_{LMj_1m_1}^{jm} = \oint d\Omega \Omega_{j\ell m}^+ Y_{LM}^{(\vec{n})} \Omega_{j_1\ell_1 m_1}^{(\vec{n})}, \tag{14}$$

i.e.

$$A(j\ell; \text{EL}; j_1\ell_1) = \left[\frac{(2L+1)(2\ell_1+1)(2j_1+1)}{4\pi} \right]^{1/2} C_{L0\ell_1 0}^{\ell_0} W\left(L\ell_1 j \frac{1}{2}; \ell j_1\right), \tag{15}$$

and for the magnetic multipole ML

$$\begin{aligned}
A(j\ell; \text{ML}; j_1\ell_1) C_{LMj_1m_1}^{jm} &= \\
&= - \oint d\Omega_n \Omega_{j\ell m}^{+(\vec{n})} \left(\begin{matrix} \rightarrow & \rightarrow & \vec{n} \\ \sigma & Y & LLM \end{matrix} \right) (\sigma n) \Omega_{j_1\ell_1 m_1}^{(\vec{n})},
\end{aligned} \tag{16}$$

i.e.

$$A(j\ell; \text{ML}; j_1\ell_1) = [L(L+1)]^{-1/2} [j(j+1) - j_1(j_1+1) + \ell'_1(\ell'_1+1) - \ell(\ell+1)] A(j\ell; \text{EL}; j_1\ell_1). \tag{17}$$

Here, $\ell'_1 = 2j_1 - \ell_1$; $W(abcd;ef)$ is the Racah coefficient; $\vec{\sigma}$ the Pauli matrices.

3. Tabulated in the paper are the one-electron conversion coefficients $w_e(\Lambda L[n\ell j]^\dagger \hbar\omega)$ for a number of selected ΛL transitions of atomic nuclei with energies $\hbar\omega \lesssim 3$ keV. Generally, the partial ICCs are used to characterize the conversion process and are tabulated in a wide region

of change of the Z (charge of the nucleus), ΛL and $\hbar\omega$ parameters (see, for example, the tables of this type in Ref. [21]). This paper, however, studies the individual ΛL nuclear transitions in the low-energy region $\hbar\omega \approx 3$ keV. As noted, the conversion probability, represented by the coefficients $w_e(\Lambda L[n\ell j]^1 \hbar\omega)$, is of direct physical relevance for these transitions. It is convenient to use these coefficients for the case when filling of the outer orbits of the atomic shell during immersion in a medium varies greatly depending on the atom's chemical environment. As shown in Ref. [8], change in the intensity of the strong conversion lines of about 1% and more allows direct interpretation in terms of change in amplitude of the electron orbit wave functions in the conversion zone. To carry out such an interpretation of the data, reference conversion coefficients are also required.

Summary of the selected nuclear transitions

1. In the nuclear excitation energy region $E^* \leq 1$ MeV, pairs of close levels $E_1 I_1$ and $E_2 I_2$ with a difference $E_1 - E_2 \lesssim 3$ keV are found in nuclear spectra quite frequently. However, fairly intensive conversion transitions with this energy are very rarely observed. If the main aim is subsequent use of the low-energy nuclear ΛL multipole conversion process to study the dependence of the atomic electron shell structure on the chemical environment (conversion method), then it is necessary to have as wide a range as possible of nuclei with observed weak transitions of varied multipolarity. To this end, an initial search was carried out for such possible transitions in the available range of nuclei and cases were selected in which such transitions have been observed, or where at first glance, there is reason to believe that they might be observed and able to compete with the other decay channels of the isomeric nuclear level. Until a detailed (model) analysis of the competitiveness of the selected transitions is carried out (that is a task for the future), the authors have limited themselves to the energy region $\hbar\omega \lesssim 3$ keV, although it is already obvious that the isomer energy range $\hbar\omega$ needs to be extended to about 5–10 keV so as to increase significantly the range of isomers that can be used in experiment which have formation conditions (yield, sample purity, definiteness of the compound's chemical structure, etc.) that satisfy the demands of the conversion spectroscopy method. Currently two isomers are widely used in the conversion method: ^{235m}U and ^{99m}Tc . The inclusion of each new isomer in the study is a key moment in developing a new method of research into matter.

2. All the selected nuclei are split into two groups — A and B, according to the isomeric transition position in the spectrum of nuclear states: in group A the isomeric level is very close to the ground state of the nucleus and transition is to the ground state; in group B the measured transition takes place between excited states of the nucleus and there is a possibility of competition with stronger transitions, in particular to the ground state.

In situation A, we need to look for processes with the most effective population of the isomeric level, while in situation B we still need to evaluate the competitiveness of the useful isomeric transition $E_1 I_1 \rightarrow E_2 I_2$ vis-à-vis other concomitant level $E_1 I_1$ channels of decay to the ground state of the nucleus or to all other levels lying between the ground state and level $E_2 I_2$. Since in these concomitant transitions considerably more energy is involved than in the isomeric one, an isomeric transition with $\hbar\omega = E_1 - E_2 (\lesssim 3$ keV) can be competitive only if specific conditions are fulfilled; when more energetic transitions are significantly hindered, for example owing to greater multipolarity than in the isomeric transition, or because of structural features of the nuclear states, for example ΔK -change forbiddenness of the

momentum projection to the symmetry axis of a strongly deformed nucleus, or configuration forbiddenness, etc.

3. A summary of selected group A transitions is given in Table 1 and for group B in Table 2. The one-electron conversion coefficients $w_e(\Lambda L[n\ell j]^1 \hbar\omega)$ of the corresponding multipole in shells of an isolated, free atom are tabulated for all these transitions. For a given population $N(n\ell j)$ of electron $(n\ell j)$ orbits, these tables can be used to find the full conversion probability in $(E_1 I_1 \rightarrow E_2 I_2)$ transition of a nucleus:

$$W_{\text{conv}}(\Lambda L; I_1 \rightarrow I_2; \hbar\omega) = e^4 m / \hbar^3 (R_0 / a_0)^{2L} \left(\frac{2I_2 + 1}{2I_1 + 1} \right) \left| \langle I_2 \| \Lambda L \| I_1 \rangle \right|^2 \xi(\Lambda L).$$

Here, the full conversion coefficient of a ΛL multipole is introduced:

$$\xi(\Lambda L) = \sum_{(n\ell j)} N(n\ell j) w_e(\Lambda L[n\ell j]^1 \hbar\omega),$$

where summation is with respect to the band orbitals in which the conversion process is energetically allowed, i.e.:

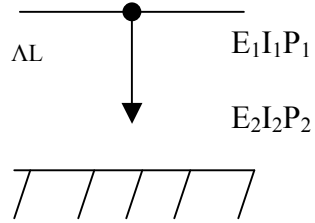
$$\hbar\omega > [mc^2 - \varepsilon(n\ell j)] = E(n\ell j)$$

where $\varepsilon(n\ell j)$ is the full (relativistic) energy of the bound electron; $E(n\ell j)$ is the binding energy.

Since the energies of the nuclear levels and nucleus transitions $\hbar\omega$ are known with errors that vary greatly in magnitude for the different possible cases investigated in groups A and B, for all the selected transitions calculations have been made for successive energy values $\hbar\omega_i$ filling an interval which is fixed by the experimental error ($\pm\Delta\hbar\omega$) around the centre. The authors did not try to standardize the calculation procedure for the whole series of selected nuclei; each case was examined individually; the number of $\hbar\omega_i$ points in the $\pm\Delta\hbar\omega$ interval varied between 10 and 20, each interval $2\Delta\hbar\omega$ having its own step $\delta\hbar\omega$. For each nuclei group, the steps $\delta\hbar\omega$ vary quite widely according to the $\Delta\hbar\omega$ magnitude. The step size is shown in Tables 1 and 2, along with the energy interval limits of the $\hbar\omega$ transition in which the one-electron conversion coefficients are calculated.

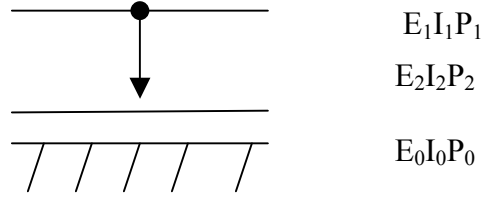
4. The case of the uniquely weak E3 transition of $^{235\text{m}}\text{U}$ ($\hbar\omega = 76.8 \pm 0.5$ eV, [4]) has been studied in close detail and since the results are given in Refs [8, 11, 12] the isomer $^{235\text{m}}\text{U}$ has not been included below. The special case of threshold behaviour of conversion coefficients for the isomer $^{90\text{m}}\text{Nb}$ is examined in detail in [8]. These results are not included here.

Table 1. Group A nuclei - isomeric level close to the ground state of the nucleus.



Nucleus	Transition $I_1P_1 \rightarrow I_2P_2$	ΔL	Energy interval $\leq \hbar\omega \leq$, keV	Step $\delta\hbar\omega$, eV	Reference
$^{103}\text{Ru}_{44}$	$5/2^+ \rightarrow 3/2^+$	M1+E 2	2.500-2.900	40	[22]
$^{110}\text{Ag}_{47}$	$2^- \rightarrow 1^+$	E1	1.080-1.140	4	[23]
$^{142}\text{Pr}_{59}$	$5^- \rightarrow 2^-$	M3+E 4	3.650-3.710	4	[24]
$^{193}\text{Pt}_{78}$	$3/2^+ \rightarrow 1/2$	M1+E 2	1.630-1.660	3	[25]
$^{201}\text{Hg}_{80}$	$1/2^- \rightarrow 3/2^-$	M1+E 2	1.500-1.650	15	[26]
$^{205}\text{Pb}_{82}$	$1/2^- \rightarrow 5/2^-$	E2	2.200-2.600	40	[27]
$^{236}\text{Pa}_{91}$	$(0^-) \rightarrow (1^-)$	M1	1.900-2.100	13	[28]
$^{235}\text{U}_{92}$	$1/2^+ \rightarrow 7/2^-$	E3	76.8 ± 0.5 eV	-	[4]

Table 2. Group B nuclei - isomeric level not close to the ground state of the nucleus.



Nucleus	E_1 , keV	Transition $I_1 P_1 \rightarrow I_2 P_2$	ΔL	Energy interval $\leq \hbar\omega \leq$, keV	Step $\delta\hbar\omega$, eV	Reference
$^{90}\text{Nb}_{41}$	124.8	$4^- \rightarrow 6^+$	M2+E 3	2.00-2.800	40	[29]
$^{99}\text{Te}_{43}$	142	$1/2^- \rightarrow 7/2^+$	E3	2.082-2.182	10	[30]
$^{110}\text{Ag}_{47}$	118.65	$3^+ \rightarrow 6^+$	M3	1.200-1.350	10	[31]
$^{140}\text{Pr}_{59}$	29.5	$3^+ \rightarrow 2^+$	M1+E 2	2.050-2.350	20	[32]
$^{153}\text{Gd}_{64}$	95.2	$9/2^+ \rightarrow 7/2^-$	E1	1.650-1.950	20	[33]
$^{159}\text{Gd}_{64}$	122.0	$7/2^- \rightarrow 7/2^+$	E1	2.850-3.150	20	[34]
$^{160}\text{Tb}_{65}$	139.47 3	$2^- \rightarrow 1^+$	E1	0.715-0.760	3	[35]
$^{165}\text{Tm}_6$	161.2	$7/2^- \rightarrow 7/2^+$	E1	1.800-2.400	25	[36]
$^{171}\text{Lu}_{71}$	72.9	$5/2^- \rightarrow 1/2^-$	E2	1.300-2.200	50	[37]
$^{171}\text{Lu}_{71}$	208.1	$1/2^+ \rightarrow 3/2^-$	E1	1.300-2.200	50	[37]
$^{183}\text{W}_{74}$	309.49 1	$(11/2^+) \rightarrow 9/2^-$	E1	0.515-0.575	4	[38]
$^{183}\text{W}_{74}$	208.80 4	$3/2^- \rightarrow 7/2^+$	E2	1.785-1.800	1	[38]
$^{188}\text{Re}_{75}$	172.07	$6^- \rightarrow 3^-$	M3- E4	2.607-2.647	4	[39]
$^{250}\text{Bk}_{97}$	35.4	$(4^+) \rightarrow (3^-)$	E1	0.950-1.250	20	[40]

Table 3. Electron conversion coefficients of the niobium isomer.

TRANSITION	NR 7=41 (KR) (4D3/2) (531/2) (M2																
	N	I	2	3	3	2	1	0													
N L J I 2D1/2	2P3/2	3S1/2	3P1/2	3P3/2	3D3/2	3D5/2	4S1/2	4P1/2	4P3/2	4D3/2											
E1(EV)	2467.	2369.	455.9	375.1	359.1	214.6	211.6	63.36	40.49	38.24	5.861										
k_{ω} (KEV)	2.000	2.040	2.080	2.120	2.160	2.200	2.240	2.280	2.320	2.360	2.400	2.440	2.480	2.520	2.560	2.600	2.640	2.680	2.720	2.760	2.800
ME(NLJ _{th} ω)/10 ⁴ N																					
	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	4.265	4.274	4.284	4.294	4.303	4.313	4.323	4.332	4.342	4.352	4.362	4.371	4.381	4.390	4.400	4.410	4.420	4.429	4.439	4.449	4.458
	1.232	1.247	1.263	1.278	1.293	1.308	1.324	1.339	1.354	1.370	1.385	1.400	1.415	1.431	1.446	1.461	1.477	1.492	1.507	1.522	1.538
	1.650	1.650	1.650	1.650	1.650	1.651	1.651	1.651	1.651	1.651	1.651	1.652	1.652	1.652	1.652	1.652	1.652	1.653	1.653	1.653	1.653
	1.817	1.816	1.814	1.813	1.811	1.810	1.808	1.807	1.805	1.804	1.802	1.801	1.800	1.798	1.797	1.795	1.794	1.793	1.791	1.789	1.788
	1.591	1.591	1.592	1.592	1.593	1.593	1.594	1.594	1.595	1.595	1.596	1.596	1.597	1.597	1.597	1.598	1.598	1.599	1.599	1.600	1.600
	7.1231	7.1267	7.1283	7.1299	7.1315	7.1331	7.1340	7.1364	7.1388	7.1394	7.1412	7.1420	7.1444	7.1460	7.1476	7.1492	7.1508	7.1524	7.1540	7.1557	7.1573
	1.072	1.094	1.095	1.097	1.097	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098	1.098
	2.355	2.355	2.356	2.356	2.356	2.356	2.356	2.357	2.357	2.357	2.357	2.357	2.358	2.358	2.358	2.358	2.358	2.359	2.359	2.359	2.359
	1.383	1.382	1.381	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380	1.380

Tables of one-electron conversion coefficients

1. The one-electron conversion coefficients $w_e(\Lambda L [n\ell j]^1 \hbar\omega)$ were calculated using formulas (1)–(17), i.e. within the framework of the so-called “no-penetration” model, [18]. The wave functions of the atomic shell were calculated using the HFS(L) method, [16, 41]. All the wave functions of both the discrete and continuous electron spectra were found by means of numerical integration of the Dirac equation with the same average atomic potential. This potential was obtained when self-consistency occurred for one of the conversion coefficients shown in the tables (see, for example, Table 3) using the population figures of the $(n\ell j)$ orbits of the electron shell configuration. All the electron functions used therefore automatically satisfy the condition of orthogonality; the energy of the escaping electron was determined using the theoretical binding energy of an orbit in the central field, i.e. $\varepsilon = \hbar\omega + mc^2 - E_i$.

Also found in this central field of the configuration identified were the functions of the unpopulated orbits, which were then used to calculate the one-electron conversion coefficients for these empty orbits. These coefficients allow a rough evaluation of the scale of the effect of the chemical environment $\delta\lambda/\lambda$ by varying the valence band configuration of the atom. It should be borne in mind that such a simplified evaluation of the $\delta\lambda/\lambda$ effect is, strictly speaking, inconsistent and can be considered only as preliminary and approximate in research into the effect; it was specifically for this purpose that the coefficients for the empty orbits were calculated since an exhaustive search of all the possible configurations (as performed for uranium and niobium) is very time-consuming.

2. ICC calculations were carried out to check the programs for calculating the one-electron conversion coefficients, and their results agreed within the given accuracy limits with both Hager and Seltzer’s well-known tables [21] and the results of the RAINE program package [16] for a series of selected points.

3. The tables of conversion coefficients $w_e(\Lambda L [n\ell j]^1 \hbar\omega)$ were calculated with a mathematical accuracy of 0.01%. We stress that this calculation accuracy has absolutely no bearing on the physical accuracy, as the accuracy of the physical assumptions concerning the type of atomic wave functions is much lower.

4. Description of the conversion coefficient tables based on the example of Table 3:

The first line of each table heading identifies the atomic wave functions: the charge of the nucleus Z and the electron configuration in which the self-consistency was performed; the configuration is given using the $(n\ell j)$ orbit population numbers. The usual atomic notation for the electron $(n\ell j)$ orbitals was used (s, p, d, f states). Next, the multipolarity of the nuclear transition (EL or ML) is shown.

The first line of the table identifies the electron orbitals for which one-electron conversion coefficients have been calculated. The second line of the table contains the calculated orbital ionization energies in electron-volts. To save space, the exponents of the conversion coefficients have been entered in the third line (denoted as N). Thus, the tables do not show the conversion coefficients themselves but the values normalized by means of multiplication by 10^{-N} . The column on the far left of the table contains the nucleus transition energies $\hbar\omega$ (in kilo-electron-volts) used to calculate the conversion coefficients.

The conversion coefficient for the M2 transition of ^{90m}Nb ($Z=41$) was calculated with atomic

functions obtained by means of self-consistency for the given electron configuration: $\{\text{Kr}\}4d3/2^4(5s1/2)^1$ shown in the heading, whereby the one-electron coefficient of the M2 multipole at the point $\hbar\omega = 2.44$ keV is $w_e(M2[4s1/2]^1 \hbar\omega = 2.44 \text{ keV}) = 7.428 \cdot 10^2$.

The binding energy of the (4s1/2) orbital in the HFS(L) approximation is 63.36 eV. In these calculations, the value taken for the exchange term parameter of the potential energy of an electron in the atomic field is $C=1$; the orbit binding energy $E(n\ell j)$ can be compared with the calculation results in Ref. [42] carried out using the same scheme.

REFERENCES

1. EMERY G.T., Ann. Rev. Nucl. Sci., 1972, v.22, p.165.
2. DRAGON O., Advances in Electronics and Electron Physics, 1983, v.60, p.1.
3. NEVE DE MEVERGNIES, M. Phys. Rev. Letters, 1972, v.29, p.1188; 1969, v.23, p.442; Phys. Letters B, 1974, v.49, p.428.
4. ZHUDOV V.I., ZELENKOV A.G., KULAKOV V.M., et al., Pis'ma v ZhEhTF, 1979, v.30, p.549.
5. ZHUDOV V.I., KULAKOV V.M., ODINOV B.V., PANOVA A.D., Voprosy atomnoj nauki i tekhniki, Ser.: Yadernye konstanty, 1984, No. 4(56), p.3.
6. MAZAKI H., KAKIUCHI S., MUKOYAMA T., MATSUI M., Phys. Rev. C, 1980, v.21, p.344.
7. MEYKENS A., FETTWEIS P., NEVE DE MEVERGNIES M., Z.Phys. A, 1978, v.284, p.417.
8. GRECHUKHIN D.P., SOLDATOV A.A., Voprosy atomnoj nauki i tekhniki, Ser.: Yadernye konstanty, 1984, No. 2(56), p.36.
9. SLATER J.C., Phys. Rev., 1951, v.84, p.1261.
10. BAND I.M., SLIV L.A., TRZHASKOVSKAYA M.B., Nucl. Phys. A, 1970, v.156, p.170.
11. GRECHUKHIN D.P., SOLDATOV A.A., Yadernaya Fizika, 1976, v.23, p.273.
12. GRECHUKHIN D.P., SOLDATOV A.A., Ibid., 1983, v.38, No. 6(12), p.1397.
13. GRECHUKHIN D.P., ZHUDOV V.I., ZELENKOV A.G., et al., Pis'ma v ZhEhTF, 1980, v.31, p.627.
14. GERASIMOV V.N., ZELENKOV A.G., KULAKOV V.M., et al., Zhurnal eksperimental'noj i teoreticheskoj fiziki, 1982, v.82, p.362; 1984, v.86, p.1169; Yadernaya Fizika, 1981, v.34, p.3.
15. SOLDATOV A.A., Preprint IAEh-3916/I, Moscow, 1984; Voprosy atomnoj nauki i tekhniki, Ser.: Obshchaya i yadernaya fizika, 1984, No. 4(29), p.86.
16. BAND I.M., LISTENGARTEN M.A., TRZHASKOVSKAYA M.B., FOMICHEV V.I., Preprint LIYaF-289, Leningrad, 1977.
17. AKHIYEZER A.I., BERESTETSKIY V.B., Quantum Electrodynamics, Moscow, Nauka, 1969 [in Russian].
18. BAND I.M., LISTENGARTEN M.A., FERESIN A.P., Anomalies in Internal Gamma Ray Conversion Coefficients, Leningrad, Nauka, 1976 [in Russian].
19. BOHR O., MOTTELSON B., The Structure of an Atomic Nucleus, v.1,2, Moscow, Mir, 1971 [in Russian].
20. ALDER K., BOHR O., HUUS T., et al., Study of the Structure of a Nucleus during Coulomb Ion Excitation. In the book "Deformation of Atomic Nuclei", edited by L.A. Sliv, Moscow, Izd-vo inostr. lit., 1958 [in Russian].
21. HAGER R.S., SELTZER E.C., Nucl. Data, 1968, v.A4, p.1.
22. BARTSCH H., HUBER K., et al. Nucl.Phys. A, 1975, v.252, p.1.

23. CLARK D.D., KOSTROUN V.O., SILMS N.E., Phys. Rev. C, 1975, v.12, p.595.
24. BERCKS C., HUMMEL E., SCHEDL K.H., Z.Phys. A, 1975, v.273, p.385.
25. ALL I. SALEH, BRAGA R.A., FINK R.W., Ibid., 1976, v.279, p.27.
26. HOFMANN S., WALCKER D., Ibid., 1975, v.272, p.351.
27. HAMILTON J.H., ANANTHAKRISHNAN V., et al., Phys. Rev. C, 1972, v.6, p.1265; Jardine L.J., Shihab-Eldin A.A., Ibid. 1976. v.13, p.348.
28. ORTH C.J., DANIELS W.R., DROPECKY B.J., Ibid., 1973, v.8, p.2364.
29. SERDUKE F.J.D., LAWSON R.D., GLOECKNER D.H., Nucl.Phys. A, 1976, v.256, p.45.
30. CHOPRA R.C., TANDOM P.H., DEVARE S.H., DEVARE H.G., Ibid., 1973, v.209. p.461; Nucl. Data Sheets, 1974, v.12, N 4.
31. BERTSCHAT H., LEITHÄUSER U., LEITZ W., et al. Nucl. Phys. A, 1974, v.229, p.72.
32. SCHEDL K.H., BERCKS C., Hummel E. Z.Phys. A, 1975, v.272, p.417.
33. Nucl. Data Sheets, 1973, v.10, N 5.
34. Ibid., v.3, N 5.
35. KERN J., MAURON G., MICHAUD B., et al., Nucl.Phys. A, 1974, v.221, p.333.
36. TAMURA T., REZANKA I., IWATA S., et al., Phys. Rev. C, 1973, v.8, p.2425; Nucl. Data Sheets, 1974, v.11, N 2.
37. Nucl. Data Sheets, 1974, v.11, N 4; Schilling K.D., Käubler L. et al. Nucl. Phys. A, 1976, v.265, p.58.
38. Nucl. Data Sheets, 1975, v.16, N 2.
39. Ibid., 1973, v.10, N 6; Shere E.B., Gruber U., Maier B.P.K. et al. Phys. Rev. C, 1972, v.6, p.537.
40. Nucl. Data Sheets, 1976, v.17, N 3.
41. Latter R. Phys. Rev., 1955, v.99. P.510.
42. BAND I.M., TRZHASKOVSKAYA M.B., Preprint LIYaF-90.91.92, Leningrad, 1974.

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