Applied Radiation and Isotopes 109 (2016) 177–182

Contents lists available at ScienceDirect

Applied Radiation and Isotopes

journal homepage: www.elsevier.com/locate/apradiso

Systematic comparison of beta spectra calculations using improved analytical screening correction with experimental shape factors

X. Mougeot

CEA, LIST, Laboratoire National Henri Becquerel, Gif-sur-Yvette F-91191, France

HIGHLIGHTS

- Analyzed database of experimental shape factors from measured beta spectra.
- Classical and improved beta spectra calculations have been implemented.
- Theoretical and measured beta spectra were systematically compared.
- The assumption $\lambda_k=1$ is inappropriate for all forbidden unique decays.
- The ξ-approximation is incorrect for half of first forbidden non-unique decays.

ARTICLE INFO

Article history:
Received 9 April 2015
Accepted 19 November 2015
Available online 27 November 2015

Keywords:
Radionuclide metrology
Decay data
Beta spectrometry
Shape factors
Beta spectrum calculation
Beta mean energy

ABSTRACT

From a review of the available literature, a database of experimental shape factors from measured beta spectra was created in previous work. Classical assumptions applied in beta spectra calculations which avoid the determination of the electron and nuclear wave functions were tested by comparison with each measured spectrum present in the database. From this systematic comparison, it was demonstrated that the typical assumption $\lambda_k=1$ is inappropriate for all forbidden unique transitions. Moreover, the equally common ξ-approximation was also proved to be incorrect for about half of the listed first forbidden non-unique transitions and for all second non-unique ones. In present work, this study has been performed once again using an improved analytical screening correction. General results from previous study still remain the same. Except for allowed transitions, the mean energies in current nuclear databases are expected to be erroneous. Some selected beta spectra are also given to illustrate these results.

1. Introduction

As an active member of the DDEP working group (Helmer et al., 2002), the National Laboratory Henri Becquerel (LNE-LNHB) evaluates decay data for improving the fundamental knowledge of decay schemes of radionuclides, thus fulfilling needs of the end user community and supporting radionuclide metrology in particular. Beta emission properties, such as the shape of the energy distribution of the emitted beta particle, are crucial features and more precise studies are required to improve experimental data and theoretical modeling.

In radionuclide metrology, beta spectra are needed e.g. for the modeling of the light emission in activity measurements carried out by the Liquid Scintillation Counting (LSC) techniques using the triple to double coincidence ratio (TDCR) method or the CIEMAT/NIST method (Broda et al., 2007).

Currently, various assumptions are usually applied for performing simple, but fast, analytical calculations of beta spectra. To test the validity of these assumptions, a systematic comparison of the calculations with experimental shape factors was performed in previous work (Mougeot, 2015). A database of 130 measured beta transitions was created for this purpose and is detailed in Mougeot (2015). In the present publication, identical calculations have been performed but with an improved analytical screening correction, and the systematic comparison with experimental shape factors has been performed once again to test their reliability. These calculations are briefly summarized, highlighting also the $\lambda_k=1$ approximation when dealing with forbidden unique transitions and the ξ-approximation for forbidden non-unique ones. These two approximations drastically simplify the calculation of the theoretical shape factor, defined in Section 2.1 Eq. (3), in order to avoid calculating the electron and nuclear wave functions.

More complex calculations have already been carried out in previous work but they were focused on the precise evaluation of

E-mail address: xavier.mougeot@cea.fr

http://dx.doi.org/10.1016/j.apradiso.2015.11.030
0969-8043/

atomic effects in allowed transitions (Mougeot and Bisch, 2014). The present comparison concentrates on the two main assumptions currently applied that have a huge impact on beta spectrum shapes, but which are used beyond their range of application (Huber, 2011). Present calculations are more refined than the usual ones mainly because the λ_k parameters, defined in Eq. (4), can be exactly calculated. It is therefore possible to clearly confirm or disprove the accuracy of the $\lambda_k=1$ approximation. However, for forbidden non-unique decays a simple method for determining the beta spectra cannot be defined. Therefore, the validity of the ξ-approximation can only be tested through a systematic comparison with measurements.

Present calculations are described in Section 2. Analysis parameters and results from the systematic comparison are summarized in Section 3. A selection of important beta spectra for LSC are shown in Section 4 to illustrate the applicability of the usual approximations.

2. Calculations

Some quantities used throughout this work are defined below:

- α is the fine structure constant,
- m_e is the electron rest mass,
- Z and A are the daughter nuclide atomic and mass numbers respectively,
- R is the nuclear radius,
- E is the kinetic energy of the beta electron,
- $W=1+E/m_e$ is the total energy of the electron including rest mass,
- E_0 and W_0 are the corresponding maximum energies,
- $p=\sqrt{W^2-1}$ is the beta particle momentum,
- $q=W_0-W$ is the corresponding momentum of the (anti)neutrino particle.

2.1. Spectrum shape

Due to the three-body nature of beta decay, the energy spectrum of the emitted beta particles is continuous. The spectrum shape is built from three meaningful parts: (i) a phase space factor pWq^2 that shares the momentum between the beta and neutrino particles; (ii) the Fermi function $F(Z,W)$ which takes into account the static Coulomb corrections due to the electromagnetic field of the nucleus; and (iii) a shape factor $C(W)$ which comes from the coupling between the nuclear structure and the lepton dynamics. Behrens' formalism (Behrens and Bühring, 1982) was followed throughout this work, using natural units $\hbar=m_e=c=1$, where (anti-)neutrinos are assumed to be massless. The shape of a beta spectrum is then

$$\frac{dN}{dW}\propto pWq^2F(Z,W)C(W) \tag{1}$$

It should be noted that in Behrens' formalism the Fermi function used, $F(Z,W)$, results from the product of the usual Fermi function F_0 and a factor L_0 which accounts for the distortion of the electron wave function by a non-point-like nuclear charge

$$F(Z,W)=F_0L_0=\frac{\alpha_{-1}^2+\alpha_1^2}{2p^2} \tag{2}$$

Thus, $F(Z,W)$ as used here already includes the finite nuclear size effect through L_0. As shown in Eq. (2), this specific Fermi function is calculated from the Coulomb amplitudes α_k of the electron wave functions. Their evaluation is described in detail in Mougeot (2015). Notice that with this definition, the calculation of the Fermi function depends neither on the method used to determine the wave functions nor on the structure of the Coulomb potential.

A beta decay occurs from an initial nuclear state of the parent nucleus with spin and parity (J_i,π_i) to a final nuclear state (J_f,π_f) of the daughter nucleus. The transition is classified on account of the spin change $|\Delta J|=|J_i-J_f|$ and the parity change $\pi_i\pi_f$. It has already been demonstrated in Behrens and Bühring (1982) that for allowed and forbidden unique transitions, the nuclear structure does not influence the energy dependence of the theoretical shape factor $C(W)$. Given that $L=1$ if $\Delta J=0$ for an allowed transition, and $L=\Delta J$ for any $(L-1)$th forbidden unique transition, the theoretical shape factor is

$$C(W)=(2L-1)!\sum_{k=1}^{L}\lambda_k\frac{p^{2(k-1)}q^{2(L-k)}}{(2k-1)![2(L-k)+1]!} \tag{3}$$

The λ_k parameters are defined from the Coulomb amplitudes α_k

$$\lambda_k=\frac{\left(\alpha_{-k}^2+\alpha_k^2\right)}{\left(\alpha_{-1}^2+\alpha_1^2\right)} \tag{4}$$

Precise calculation of the electron wave functions, and thus of α_k and λ_k, is not straightforward. A usual assumption is to set $\lambda_k=1$ to avoid calculating these parameters because their energy variation can be weak for certain transitions. This assumption is referred to as the $\lambda_k=1$ approximation in the present work.

Nuclear structure effects cannot be avoided when considering forbidden non-unique transitions, and no simple formulation such as the one given in Eq. (3) can be established. However, theoretical arguments exist to justify that *some first* forbidden non-unique transitions can be calculated as allowed if the Coulomb energy of the emitted beta particles at the nuclear surface is much higher than the maximum energy of the transition, which is referred to as the ξ-approximation (Schopper, 1966)

$$2\xi=\frac{\alpha Z}{R}\gg E_0 \tag{5}$$

Given the difficulty of determining the forbidden non-unique beta spectra, the ξ-approximation is usually extended to *all* non-unique transitions, calculating a forbidden non-unique transition as a forbidden unique one with identical ΔJ.

2.2. Corrections

A final modification is also applied to the spectrum shape in Eq. (1) by applying the atomic screening effect, which is the only atomic effect taken into account in this work. Secondary shake-up and shake-off effects have been neglected because of their very small influence (Cooper and Åberg, 1978). However, atomic screening and exchange effects have been proved to be of great importance for a precise description of beta spectrum shapes at low energy (Mougeot and Bisch, 2014). At present, these accurate calculations can only be performed for allowed transitions, and are time consuming.

The usual simple approach from Rose (1936) was chosen in previous work (Mougeot, 2015), in which the screening effect is evaluated using a screened Thomas-Fermi potential V_0 that depends only on Z. Basically, the beta emission probability at an energy W is approximated by the probability at $W'=W-V_0$ for beta minus transitions and at $W'=W+V_0$ for beta plus transitions (Gove and Martin, 1971). It is noteworthy that evaluating the screening effect with this method leads to a non-physical discontinuity in each beta minus spectrum because a minimum energy $W=V_0$ is required for this correction to be applied. Obviously, this problem does not occur for beta plus transitions.