Theoretical calculation of internal conversion coefficients for multipole transitions in ^{88}Sr nucleus

Ali A. Alzubadi, Ali K. Abood

Physics Department, College of Science, University of Baghdad, Baghdad, Iraq

E-mail: ali.a.alzubadi@gmail.com

Abstract

Internal conversion coefficients (ICC) and electron–positron pair conversion coefficients (PCC) for multipole transition of the core nucleus ^{88}Sr have been calculated theoretically. The calculation is based on the relativistic Dirac–Fock (DF) solutions using the so called ‘‘Frozen Orbital’’ approximation, takes into account the effect of atomic vacancies created in the conversion process, covering a transition energies of 1–5000 keV**.** A large number of points were used to minimize any errors due to mesh-size effects. The internal conversion coefficients display a smooth monotonic dependence on transition energy, multipolarity and atomic shell. Comparing the values of PCC to ICC, it is interesting to note, that the energy dependence of PCC is monotonically increasing and ICC is decreasing with the transition impulses momentum. Resonance minima in the energy dependence of ICCs for the *ns* shells L1, M1 and N1 at E2–E5 transitions have been also observed.

Key words

Internal conversion coefficients,
electric and magnetic mulipole transitions.

Article info
Received: Jun. 2012
Accepted: Nov. 2012
Published: Dec. 2012

الحساب النظري لمعاملات التحول الداخلي للأنتقال متعدد الأقطاب لنواة ^{88}Sr

علي عبد اللطيف كريم الزبيدي، علي خالد عبود

قسم الفيزياء، كلية العلوم، جامعة بغداد، بغداد، العراق

الخلاصة

معاملات التحول الداخلي (ICC) و معاملات تحول الالكتروت بوزيترون (PCC) للأنبعاث متعدد الأقطاب قد تم حسابها نظريا لنواة القلب ^{88}Sr بالأعتماد على حلول ديراك-فوك النسبية و باستخدام تقريب المدار المجمد مع الأخذ بنظر الأعتبار تاثير الفجوات الذرية المتكونة خلال عملية التحول ولمدى طاقة الأنتقال 1-5000 keV. لقد تم أستخدام عدد كبير من النقاط وذلك لتقليل اي خطأ قد ينتج بسبب تاثيرات حجم التدريجات. لقد أظهرت معاملات التحول الداخلي اعتماد أحادي التوجه مع طاقة طاقة الأنبعاث، التعددية القطبية و القشرة الذرية. عند مقارنة PCC الى ICC قد لوحظ ان أعتماد الطاقة لـ PCC في حالة تزايد أحادي التوجه و ICC في تتناقص. لقد تم ملاحظة حدوث حالة الرنين في حدوده الدنيا في أعتماد ICCs على الطاقة في الأغلفة L1و M1 و N1 للأنتقالات E2–E5.

Introduction

It is well known that a detailed study of internal conversion processes yields useful information on nuclear structure. Internal conversion coefficients (ICCs) obtained by measuring both conversion electrons and gamma rays are sensitive to the transition multipolarity and are used to assign multipolarity of the transition. Since low energy and/or high-multipole transitions have large conversion coefficients, they show up strongly with respect to other transitions. Multipolarities and mixing ratios of nuclear transitions are determined by a comparison of experimental ICCs with corresponding theoretical values. These in turn are useful for the spin and parity assignments of excited nuclear states and the construction of nuclear level schemes. They have various applications such as the study of the influence of the chemical environment on atoms, Mossbauer experiments [1], nuclear reaction calculations [2] and studies of the electronic structure of condensed matter. Nuclear decay data are also extensively used in a wide range of applications, including the nuclear fuel cycle [3], environmental control, and nuclear medicine.

Theory and methodology

The conversion coefficient (α_{ic}) is defined as the ratio of the electron emission rate (T_{ic}) to the gamma emission rate ($T\gamma$):

$$\alpha_{ic} = T_{ic} / T_{\gamma} \tag{1}$$

Depending on the electron shells involved it is customary to define conversion coefficients for sub-shells (α_{L1}, α_{L1}, etc.) or for major shells (α_K, α_L, etc.). Similarly, the conversion coefficient involving electron–positron pair emission (T_π) is defined as:

$$\alpha_{\pi} = T_{\pi} / T_{\gamma} \tag{2}$$

For transitions between spin zero states of the same parity, $0_i^+ \rightarrow 0_f^+$ (or $0_i^+ \rightarrow 0_f^+$), the emission of single γ-photon is strictly forbidden by considerations of angular-momentum conservation and, therefore, a conversion coefficient is not defined. For mixed $(\pi L + \pi' L')$ multipolarity transitions the conversion coefficient can be obtained from the formula:

$$\alpha = \frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1+\delta^2} \tag{3}$$

where $\alpha(\pi L)$ and $\alpha(\pi' L')$ are the conversion coefficients for the pure multipolarity components.

The relativistic expression for ICC in the ith atomic sub–shell, derived in the framework of the first non-vanishing order of perturbation theory and one-electron approximation for a free neutral atom can be written as [4]:

$$\alpha_i^{TL} = \sum_{K_f} \left| M_i^{\tau L}(K_f) \right|^2 . \tag{4}$$

The partial conversion matrix element is $M_i^{\tau L}(K_f) = B_i^{\tau L}(K_f) R_i^{\tau L}(K_f)$, where $B_i^{\tau L}(K_f)$ is the angular part, $R_i^{\tau L}(K_f)$ is the radial part, and, and τL is the nuclear transition multipolarity of electric type $\tau = E$ or magnetic one $\tau = M$. Use is made of relativistic quantum numbers $K = (l-j)(2j+1)$, where ℓ is the electron orbital momentum, and j is the total electron momentum. Indices i and f refer to the initial (bound) and final (continuum) states of the electron, respectively.

The summation in Eq. 4 extends over all final states allowed by the selection rules

$$|L - j_i| \le j_f \le L + j_i \tag{5}$$

$$\ell_i + \ell_f + L \quad is \begin{Bmatrix} \text{even for EL transition} \\ \text{odd for ML transition} \end{Bmatrix} \tag{6}$$

For electric transitions, $B_i^{\tau L}$ and $R_i^{\tau L}$ are given by

$$B_i^{EL}(K_f) = (-1)^{j_f + \frac{1}{2} + L} C_{l_i 0 l_f 0}^{L0} W\left(l_i j_i l_f j_f ; \tfrac{1}{2} L\right) \times \left[\pi k \alpha \frac{(2j_i+1)(2l_i+1)(2j_f+1)(2l_f+1)}{L(L+1)(2L+1)} \right]^{\frac{1}{2}} \tag{7}$$

and

$$R_i^{EL}(K_f) = (K_i - K_f)\left(R_{1,\Lambda=L-1} + R_{2,\Lambda=L-1}\right) + L\left(R_{2,\Lambda=L-1} - R_{1,\Lambda=L-1} + R_{3,\Lambda=L}\right) \tag{8}$$

In Eq. 7, *k* equals *Eγ* in units of $m_o c^2$, *α* is the fine structure constant, $C^{L0}_{\ell_i 0 \ell_f 0}$ is the Clebsch–Gordan coefficient, $W\left(\ell_i j_i \ell_f j_f ; \tfrac{1}{2} L\right)$ is the Racah coefficient and for magnetic transitions, the corresponding expressions are

$$B_i^{ML}\left(K_f\right)=\left(-1\right)^{j_f+\frac{1}{2}+L} C^{L0}_{\ell_i 0 \bar{\ell}_f 0} W\left(\ell_i j_i \bar{\ell}_f j_f ; \tfrac{1}{2} L\right) \times\left[\pi k \alpha \frac{\left(2 j_i+1\right)\left(2 \ell_i+1\right)\left(2 j_f+1\right)\left(2 \bar{\ell}_f+1\right)}{L\left(L+1\right)\left(2L+1\right)}\right]^{\frac{1}{2}} \tag{9}$$

where $\bar{l}_f = 2 j_f - l_f$ and

$$R_i^{ML}\left(K_f\right)=\left(K_i+K_f\right)\left(R_{1,\Lambda=L}+R_{2,\Lambda=L}\right). \tag{10}$$

Radial integrals in Eqs. 8 and 10 are written as follows

$$R_{1,\Lambda}=\int_0^\infty G_i F_f\left(E_k\right) X_\Lambda\left(kr\right) dr, \tag{11}$$

$$R_{2,\Lambda}=\int_0^\infty F_i G_f\left(Ek\right) X_\Lambda\left(kr\right) dr, \tag{12}$$

$$R_{3,\Lambda}=\int_0^\infty \left[G_i G_f\left(E_k\right)+F_i F_f\left(E_k\right)\right] X_\Lambda\left(kr\right) dr. \tag{13}$$

Functions *G(r)* and *F(r)* are given by $G(r)=r\,g(r)$ and $F(r)=r\,f(r)$, where *g(r)* and *f(r)* are the large and small components of the radial electron wave function, respectively. In our calculations, *G* and *F* are solutions of the Dirac–Fock (DF) equations. Wave functions for the bound state *Gi* and *Fi* are calculated in the *DF* field of a neutral atom while continuum wave functions $G_f(E_k)$ and $F_f(E_k)$ are determined in the DF field of the ion with a vacancy in the shell from which the conversion electron is emitted. In calculating continuum wave functions, the conversion electron energy E_k is determined from the energy conservation relationship:

$$E_k = k - \varepsilon_i, \tag{14}$$

where ε_i is the binding energy for the *i*th atomic subshell. we use the experimental values of ε_i .

The radial part of the transition potential $X_\Lambda(kr)$ in the surface current model is written as follows [5]

$$X_\Lambda\left(kr\right)=\begin{cases} j_\Lambda(kr)\dfrac{h_\Lambda(kR_0)}{j_\Lambda(kR_0)} & \text{for } r \le R_0 \\ h_\Lambda(kr) & \text{for } r > R_0 \end{cases} \tag{15}$$

where $j_\Lambda(x)$ and $h_\Lambda(x)$ are spherical Bessel and Hankel functions, respectively. Inside the nucleus, the potential of a homogeneously charged sphere is assumed where $R_0 = 1.2 A^{1/3}\,\mathrm{fm}$ is the radius and *A* is the mass number. Eqs. 4-15 make use of relativistic units where the electron Compton wavelength $\hbar/m_0 c$ serves as unit of length and the electron rest energy $m_0 c^2$ as unit of energy.

Main calculation codes

The main calculation codes are HsIcc [5] and BrIcc V.2.3 [6]. BrIcc was adopted by the International Nuclear Structure and Decay Data (NSDD) network for all new data evaluations published in Nuclear Data Sheets and Nuclear Physics A. We used BrIcc to obtain conversion coefficients for pure and mixed multipolarity transitions for a given atomic number, transition energy, atomic shell, multipolarity and mixing ratio. The procedures are fully compliant with the Evaluated Nuclear Structure Data File (ENSDF) coding rules [7].

The main features of the data tables used by BrIcc are depends on two approximations [6], ‘‘No Hole’’ approximation, which marked as BrIccNH. In this approximation Ψ_{fin} is the Self-Consistent Field (SCF) of a neutral atom, i.e. the effect of the vacancy is disregarded. The second approximation is the ‘‘Frozen Orbitals’’, which marked as BrIccFO. This approximation also incorporates the vacancy created in the conversion process. The Ψ_{fin} is calculated in the ion potential constructed using bound wave functions of the neutral atom. The last approximation was adopted in the present research.

Results and discussion

The internal conversion coefficients for various atomic shells in ^{88}Sr have been calculated using relativistic wave functions, taking into account the finite nuclear size and shown in Figs. 1 and 2. Inspection of these Figs revels in general; the ICC is an increasing function of Z and L, and a decreasing function of E, and n.

Typically the conversion coefficients display a smooth monotonic dependence on transition energy, multipolarity, atomic shell and atomic number. In general, the ICC is decreasing with increasing transition energy. The same tendency can be seen moving towards the outer shells with the same relativistic quantum number *K*. On the other hand the ICC increases with the multipole order. However, there are deviations from the monotonic energy dependence involving $s_{1/2}$ (K, L1, M1, N1, etc.) atomic shells. These are illustrated in Fig. 1 for E1 to E5 multipolarity. For specific multipolarity and a nuclear charge, ICCs usually increase with decreasing energy Eγ. In spite of the monotonic behavior of the majority of the ICCs as a function of Eγ, it has been noted [8] that there is a minimum in $\alpha_i^{El}\left(E_\gamma\right)$ for electric transitions with $L \geq 2$. This minimum later was called as the "*ICC resonance structure*" [9, 10], which occurs at the energy E(res)γ determined by the following expression for the L1 shell [8]:

$$E_\gamma^{(res)}(keV) \approx \frac{Z^2(L-1)}{200} \qquad (16)$$

We have found [6] that there exist several minima (resonances) in $\alpha_i^{El}\left(E_\gamma\right)$ for the ns shells with $n \geq 2$, the resonance energy of Eq. (16) being the highest one.

The typical Eγ dependence of ICC for the K shell is demonstrated in Fig. 1. The curves $\alpha_i^{El}\left(E_\gamma\right)$ fall sharply near the threshold for all transitions except E1. This sharp up-bend of ICC was called "threshold non-regularity" in Ref. [6]. For light elements, the threshold non-regularities occur in ICCs only for electric transitions; however, for more heavy elements, ICC for magnetic transitions also behaves in the same way [11]. According to present calculations, ICCs for the K- shell have no resonances for all multipolarities.

As seen in Fig. 1, there is only one resonance for the L1 shell at E2–E5 transitions, but there are two resonances for the M1 and N1 shells. For various electric multipolarities, the positions of the resonances $E_\gamma^{(res)}$ shift to the right as L increases according to Eq. (16) but the general structure remains the same. For the M1 and N1 shells, new additional resonances arise at lower energies $E_\gamma \lesssim 1keV$.

The electron–positron pair conversion coefficients (PCC) in ^{88}Sr are shown in Fig. 3. Comparing PCC values to ICC it is interesting to note, that the energy dependence of PCC is monotonically increasing and ICC is decreasing with the transition impulses momentum, *L*. The energy threshold of the pair conversion process is 1022 keV.

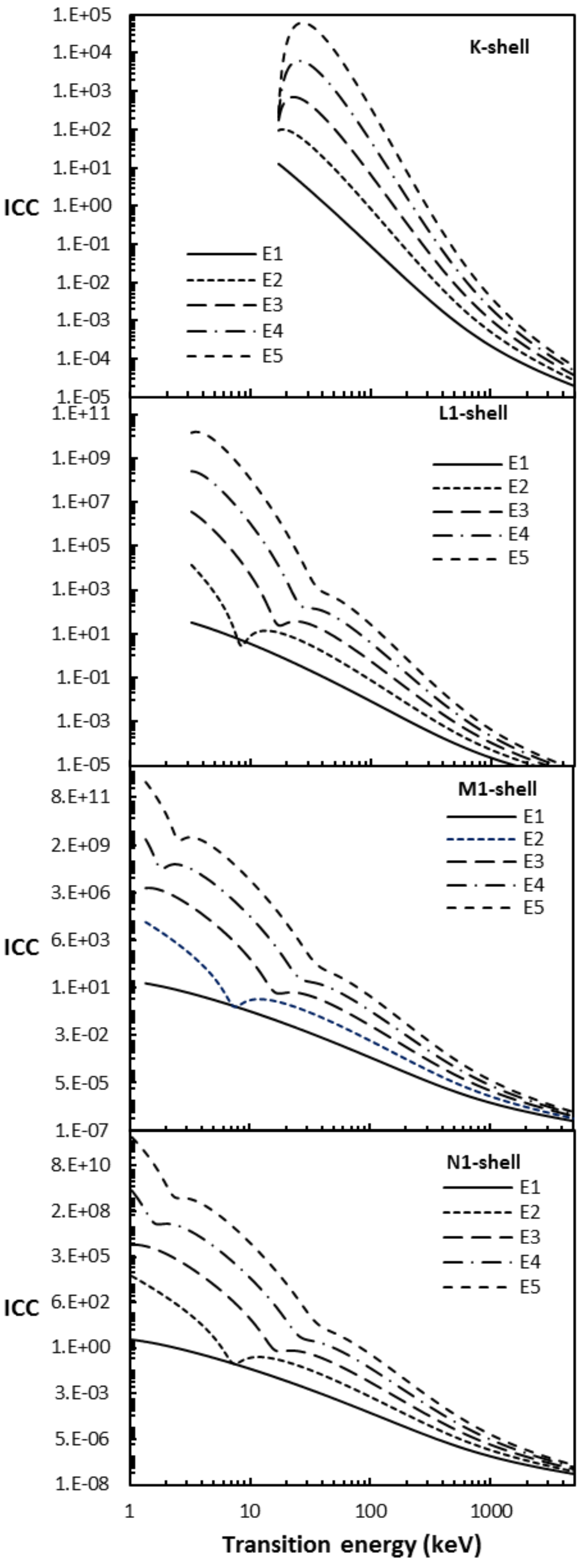

Fig.1: ICCs versus the γ -ray energy Eγ for electric multipole transition.

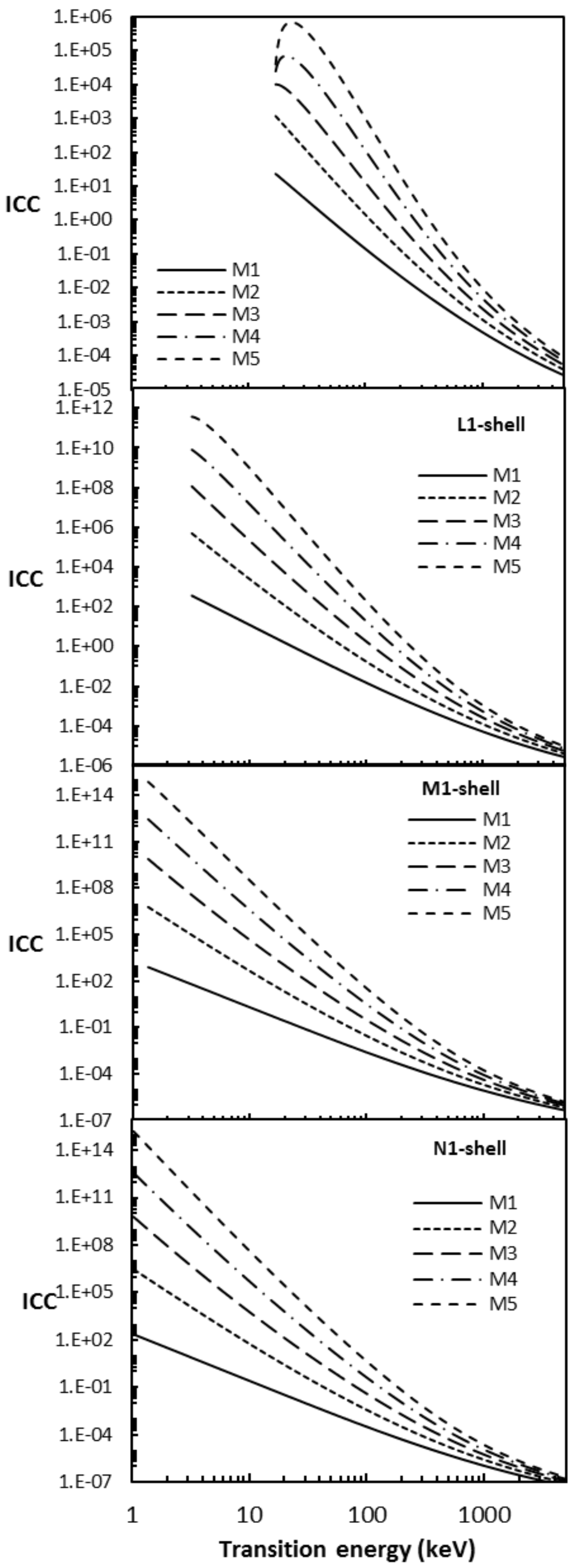

Fig.2: ICCs versus the γ -ray energy Eγ for magnetic multipole transition.

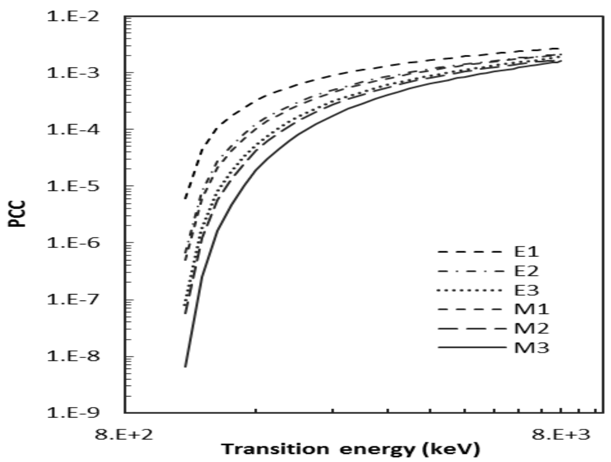

Fig.3: Electron–positron pair conversion. PCC.

The particles ejected in the electron–positron pair creation process share the available kinetic energy. The differential cross-section $d^2PCC/dE_{e^+} + d\cos\theta$ is not uniform as a function of separation angle, θ and the energy of the positron, E_{e^+} [12].

To evaluate major shell $(\alpha_L, \alpha_M, \text{etc.})$ or total (α_T) conversion coefficient interpolation could not be used in regions close to the atomic binding energies and around 1022 keV, the energy threshold of the electron–positron pair production. For ^{88}Sr, the total ICC (α_T) for electric and magnetic multipolarity are depicted in Fig.4, where the α_T values are non-continuous in these energy regions. First will interpolate the partial (subshell) values for a given transition energy using BrIcc, and then evaluated the summed values. We did not notice any unusual behavior of the total ICC. Generally, the total ICC are increasing with multipolarity, and decreasing with the transition energy. Non-monotonous energy dependence can appear near the threshold. For each atomic subshell, there is a discontinuity at its threshold energy. Note that not all of them are seen in the logarithmic scale of Fig. 4, in dependence on the relative contribution of the particular subshell to the total ICC.

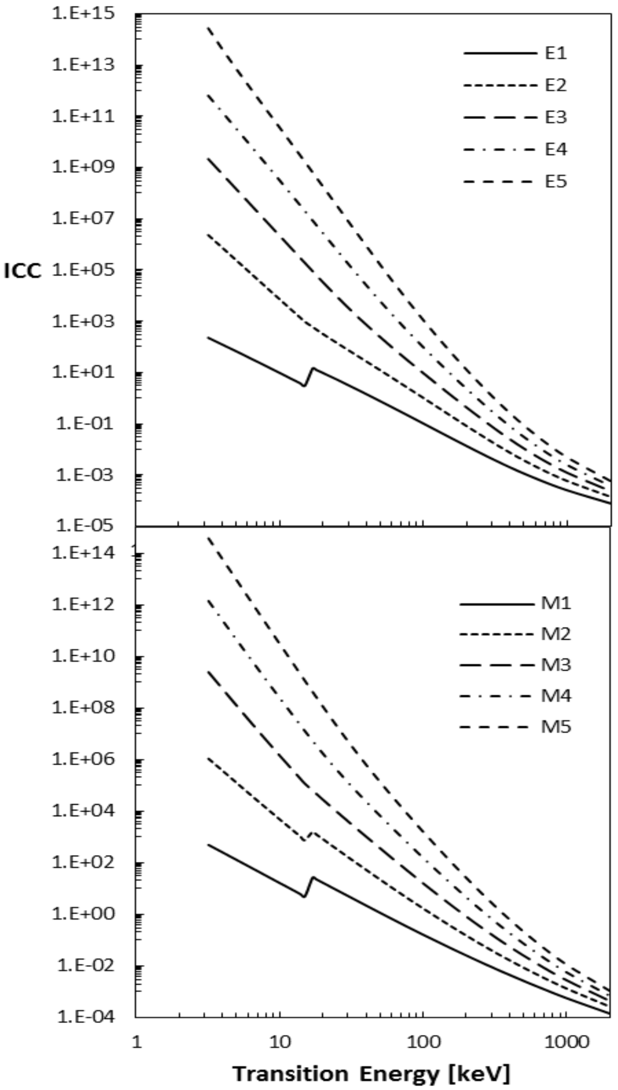

Fig.4: Total conversion coefficients. The five multipole orders (E1–E5 and M1–M5) are shown.

Conclusions

Theoretical internal conversion coefficients provide useful calibration standards for decay scheme studies. The accuracy of these conversion coefficients is sufficient to qualify them as useful calibration standards in the determination of spins and parities of nuclear levels. We have verified that the outer-shell ICC are more sensitive to treatment of the exchange interaction in the bound-electron state than are those for inner shells. Additional resonance minima have been found in the Eγ dependence of ICC at

E2–E5 transitions for the *ns* shells with $n \geq 2$ at low γ -ray energies. It is shown that ICCs may have up to four resonances for outer shells.

Acknowledgments

The authors are indebted to Prof. Dr. T. Kibedi (the writer of BrIcc code) from Australian National University for his valuable discussions and the guidance notes throughout the working in this research.

References

[1] A. Blachowski and K. Ruebenbauer, Phys. Scr. 73 (2006) 263.

[2] T. Belgya, O. Bersillon, R. Capote, T. Fukahori, G. Zhigang, S. Goriely, M. Herman, A.V. Ignatyuk, S. Kailas, A. Koning, P. Oblozinsky, V. Plujko, P. Young, Handbook for calculations of nuclear reaction data, RIPL-2, IAEA-TECDOC-1506, IAEA, Vienna, 2006.

[3] A.L. Nichols (Ed.), Beta-decay and decay heat, IAEA, INDC(NDS) 0499, (2006).

[4] I. M. Band, M. B. Trzhaskovskaya, C. W. Nestor Jr., P. O. Tikkanen, and
S. Raman, At. Data Nucl. Data Tables 81,1 (2002).

[5] S. Raman, C.W. Nestor Jr., A. Ichihara, M.B. Trzhaskovskaya, Phys. Rev. C 66 (2002) 044312.

[6] T. Kibedi, T.W. Burrows, M.B. Trzhaskovskayac, P.M. Davidsona, C.W. Nestor, Nucl. Instr. and Meth. A 589, (2008) 202.

[7] J.K. Tuli, Evaluated nuclear structure data file a manual for preparation of data sets, BNL-NCS-51655-01/02-Rev, National Nuclear Data Center, Brookhaven National Laboratory (2001).

[8] E. L. Church and J. E. Monahan, Phys. Rev. 98, (1955) 718.

[9] F. Rosel, H. M. Fries, K. Alder, and H. C. Pauli, At. Data Nucl. Data Tables 21, (1978) 91.

[10] M. B. Trzhaskovskaya, T. Kibedi, and V. K. Nikulin, Phys. Rev. C 81 (2010) 024326.

[11] T. Kibedi, M.Gupta, M.B.Trzhaskovskaya and A. E. Stuchbery, J. Korean Phys. Soci., 59, 2, (2011) 1483.

[12] C.R. Hofmann, G. Soff, J. Reinhardt, W. Greiner, Phys. Rev. C 53, (1996) 2313.