Available online at www.sciencedirect.com
ScienceDirect
Applied Radiation and Isotopes 66 (2008) 705–710
Applied Radiation and Isotopes
www.elsevier.com/locate/apradiso

# A tool for processing decay scheme data that encompasses coincidence summing calculations

Octavian Sima[a,*], Dirk Arnold[b]

[a]Physics Department, Bucharest University, Bucharest-Magurele, P.O. Box MG-11, RO-077125, Romania
[b]Physikalisch-Technische Bundesanstalt, Bundesallee 100, Braunschweig, Germany

**Abstract**

A description is given of the tool implemented in GESPECOR to process coincidence summing corrections and derive decay scheme data. The method of analysis produces relevant decay scheme data and the joint emission probability for any group of photons (gamma emissions, X-rays, annihilation photons resulting from $\beta^+$ decay) emitted in the decay of any nuclide with less than 100 levels.


*Keywords:* Decay scheme analysis; Coincidence summing; $\gamma$-Ray spectrometry

## 1. Introduction

A typical demand placed on many gamma-ray spectrometry laboratories is to maintain high spectral output while ensuring low detection limits for each sample through the use of high efficiency detectors in high efficiency measurement geometries. But this solution is convenient only if a practical method for the determination of coincidence summing corrections is possible.

The evaluation of coincidence summing effects requires an intricate combination of the decay data of the nuclide of interest and adequate detection probabilities for the emitted radiations (in the peak and in the entire spectrum). The methods applied for this purpose differ in the way in which the decay data are prepared and how the detection probabilities are evaluated and combined with the decay data. We present a complex tool applied within the GESPECOR program (Sima et al., 2001; Sima and Arnold, 2000) for preparing the necessary decay data. By separating the evaluation of the decay data from the evaluation of the efficiencies, this tool is most useful when coupled with the Monte Carlo method of efficiency evaluation, as in the case of GESPECOR. But this method of analysis is also useful in combination with other methods, because it provides insight into the relative contribution of various sets of photons to coincidence summing. The angular correlation of the photons is not implicitly included, but can easily be included if the appropriate values of the angular correlation coefficients are available.

## 2. Methods for the computation of coincidence summing corrections

The first general method for the evaluation of coincidence summing effects was proposed in 1972 (Andreev et al., 1972), and has been extended and implemented in computer programs (McCallum and Coote, 1975; Debertin and Schötzig, 1979). This approach is based on a set of recursive formulae in which the decay data and the detection efficiencies are intimately coupled. A matrix formulation was proposed by Semkow et al. (1990) and further developed by Korun and Martinčič (1993, 1995) in which the peak count rates are related to the source disintegration rate by a product of matrices that are functions of the decay scheme parameters, peak and total efficiencies. Another approach (Laedermann and Décombaz, 2000; Berlizov and Tryshyn, 2005) involves the simulation of the decay and the detection processes by means of Monte Carlo techniques. For each decay process a set of photons is selected according to the transition probabilities, and then each photon is traced through the

*Corresponding author. Fax: +40 214574521.
*E-mail address:* osima@olimp.fiz.infim.ro (O. Sima).

0969-8043/$ - see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.apradiso.2008.02.007

measurement setup. The resulting number of counts accumulated in each peak is suitably normalized and used to obtain the peak efficiency in the presence of coincidence summing effects.

The method applied in GESPECOR (Sima et al., 2001; Sima and Arnold, 2000) replaces the random sampling of the decay process by computing the joint emission probability of the various groups of photons that can be emitted simultaneously in the decay process. Then the efficiencies are evaluated by a dedicated Monte Carlo simulation. The advantages of using the computed joint emission probabilities are twofold: first, these probabilities are computed only once before the Monte Carlo simulation, saving computing time; second, the spread of the computed values of the coincidence summing corrections due to the random sampling of the decay path is eliminated. The implemented procedure represents the application of a well-known variance reduction technique, resulting in a smaller statistical spread of the results for the same number of photon histories.

## 3. Formalism: the simplest case

Consider a nuclide with $N$ levels $l = 1, 2, \ldots N$, where $l = 1$ represents the ground level and $l = N$ the highest excited level. Let $L$ be the set of all levels. Suppose that a number of transitions labeled as $j = 1, 2, \ldots$ can take place between the levels. Let $T$ be the set of all transitions. For each transition $j \in T$ we use the notation $l_i(j)$ and $l_f(j)$ to represent the initial and final level of the transition. For simplicity we shall also use the same symbol $T$ to denote the set of gamma photons emitted in the corresponding transitions, being clear from the context whether we refer to transitions or to gamma photons. The transitions (and the photons) are numbered according to the following rule: for any transitions $j$, $k \in T$ we have $j<k$ if $l_i(j) > l_i(k)$ or if $l_i(j) = l_i(k)$ and $l_f(j) > l_f(k)$. This rule is exemplified in Fig. 1 for the decay scheme of $^{134}$Cs. According to this convention a transition $k$ cannot start from a level higher than the starting levels of all the transitions $j$ with $j<k$ and cannot have the final level higher than any transitions $j$ that start on the same level with transition $k$ but have $j<k$. Furthermore, for future convenience, we define $t_i(l) \in T$ for each level $l \in L$ as the first transition starting from level $l$, i.e. $t_i(l) = \min\{j \in T | l_i(j) = l\}$; e.g. $t_i(3) = 9$ in Fig. 1.

A gamma photon can be emitted or internal conversion can take place in each transition, followed eventually by the emission of X-rays or/and Auger electrons. In order to emphasize the basic ideas, consider the simplest case, namely that we disregard the X-ray contribution to coincidence summing effects, the presence of metastable states and $\beta^+$ decay—these restrictions will be removed at a later stage.

The true coincidence summing effects which are important for spectrum analysis can be classified as coincidence losses from the peaks and coincidence

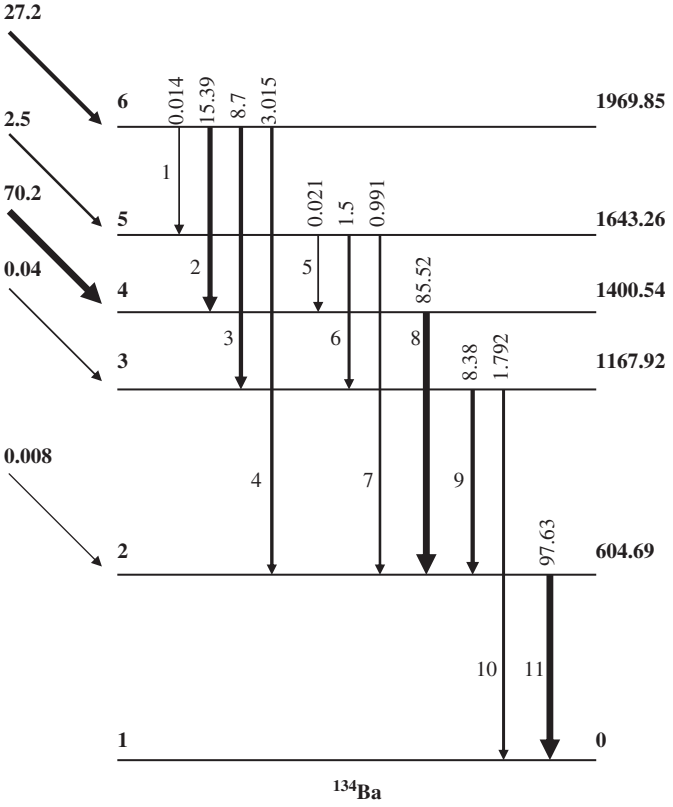


Fig. 1. $^{134}$Cs decay scheme with level and transition labeling according to the convention adopted.

contributions to sum peaks. Below we shall consider them in this order.

Let $E_i$ be the energy of the $i$th photon (i.e. photon emitted in transition $i \in T$), with absolute emission probability $p_i$. Denote by $p_{i,j}$ the probability of joint emission of the $i$th and $j$th photons, by $p_{i,j,k}$ the joint emission probability of the $i$th, $j$th and $k$th photon and so on. We consider $p_{i,j}$ as being the probability of emission of the two photons irrespective of other photons being emitted or not; for example, in the case when the triplet $\{i,j,k\}$ is emitted, this event is counted both among the cases when the pair $\{i,j\}$ is emitted and among the cases when the pair $\{i,k\}$ is emitted. Denote by $S^{(1)}(i)$ the set of photons $j \in T$ for which $p_{i,j} > 0$:

$$S^{(1)}(i) = \{j \in T | p_{i,j} > 0\}, \quad (1)$$

i.e. $S^{(1)}(i)$ represents the set of photons which can be emitted in the same decay act together with the $i$th photon. Similarly,

$$S^{(2)}(i) = \{\{j,k\} \in T | p_{i,j,k} > 0\},$$
$$S^{(3)}(i) = \{\{j,k,l\} \in T | p_{i,j,k,l} > 0\}, \quad (2)$$

and so on. For example, in the case presented in Fig. 1, $S^{(1)}(9) = \{1,3,6,11\}$, $S^{(2)}(9) = \{\{1,6\},\{1,11\},\{3,11\},\{6,11\}\}$, $S^{(3)}(9) = \{\{1,6,11\}\}$. All the photons from the sets $S^{(1)}(i)$, $S^{(2)}(i)$, $S^{(3)}(i)$ … contribute to coincidence losses from the peak associated with the $i$th photon. Indeed, if the nuclide

activity is $A$, the count rate in the peak is

$$N(E_i) = Ap_i d(i \in P) - A \sum_{j \in S^{(1)}(i)} p_{i,j} d(i \in P, j \in I) + A \sum_{j,k \in S^{(2)}(i)} p_{i,j,k} d(i \in P, j \in I, k \in I) - \cdots, \quad (3)$$

where $d$ denotes the detection probability; for example $d(i \in P, j \in I, k \in I)$ represents the probability that the complete energy of the $i$th photon has been deposited in the sensitive volume of the detector, while the $j$th and $k$th photons interacted in the sensitive volume of the detector and deposited some energy (but not necessarily their complete energy). In other words, in the absence of coincidence summing effects the $i$th photon would have been registered in the peak $P$, while the $j$th and $k$th photons would have been registered in the total (integral) spectrum I. The

$$d(i \in P) = \varepsilon_p(E_i) \quad (4)$$

is the usual peak efficiency for the energy of the $i$th photon, but the detection probability for sets of photons is usually different from the product of the corresponding peak ($\varepsilon_p$) and total ($\varepsilon_t$) efficiencies (Sima and Arnold, 2000; Arnold and Sima, 2001).

Suppose that between the initial and final levels of the $i$th transition a sequence of several linked transitions can take place, for example transitions $q \in T$ and $r \in T$ that satisfy $l_i(q) = l_i(i)$, $l_f(r) = l_f(i)$ and $l_f(q) = l_i(r)$; e.g. in Fig. 1 for $i = 10$ we have $q = 9$ and $r = 11$. Then $E_i = E_q + E_r$ and the cases when the $q$th and $r$th photons are completely absorbed into the sensitive volume of the detector without the detection of other photons add a pulse in the peak of energy $E_i$;(i.e. sum peak contributions are included in the peak count rate). We introduce the notation:

$$S^{(1)}(q,r) = \{j \in T | p_{q,r,j} > 0\},$$
$$S^{(2)}(q,r) = \{\{j,k\} \in T | p_{q,r,j,k} > 0\} \text{ and so on.} \quad (5)$$

Then the sum peak contribution of the $q$th and $r$th transition to the count rate is

$$N^{\text{sum}}(E_q + E_r) = Ap_{q,r} d(q \in P, r \in P) - A \sum_{j \in S^{(1)}(q,r)} p_{q,r,j} d(q \in P, r \in P, j \in I) + A \sum_{j,k \in S^{(2)}(q,r)} p_{q,r,j,k} d(q \in P, r \in P, j \in I, k \in I) - \cdots \quad (6)$$

Evidently, if there are more combinations of adjacent transitions starting on $l_i(i)$ and ending on $l_f(i)$, each combination will add a contribution of the same type to the sum peak. We denote the set of all these transitions by $U^{(2)}(i)$, $U^{(3)}(i)$, … where $U^{(2)}$ contains all the pairs of linked transitions, $U^{(3)}$ contains all triple linked transitions … between $l_i(i)$ and $l_f(i)$. For example, as presented in Fig. 1 $U^{(2)}(4) = \{\{1,7\},\{2,8\},\{3,9\}\}$, $U^{(3)}(4) = \{\{1,5,8\},\{1,6,9\}\}$. The final count rate in the $E_i$ peak is

$$N(E_i) = Ap_i d(i \in P) - A \sum_{j \in S^{(1)}(i)} p_{i,j} d(i \in P, j \in I) + A \sum_{j,k \in S^{(2)}(i)} p_{i,j,k} d(i \in P, j \in I, k \in I) - \cdots + \sum_{q,r \in U^{(2)}(i)} N^{\text{sum}}(E_q + E_r) + \sum_{q,r,s \in U^{(3)}(i)} N^{\text{sum}}(E_q + E_r + E_s) + \cdots, \quad (7)$$

where each $N^{\text{sum}}$ term is given by a formula similar to Eq. (6).

In the absence of coincidence summing effects [either because $S^{(1)}(i) = \varnothing$ (consequently $S^{(n)}(i) = \varnothing$ for any $n$) and $U^{(m)}(i) = \varnothing$, $m = 2, 3..$, i.e. there are no photons which can be emitted together with the $i$th photon and there are no sum peak combinations, or because the detection probabilities of the photons involved is negligible], the count rate in the same peak is

$$N^0(E_i) = Ap_i d(i \in P). \quad (8)$$

The coincidence summing correction factor for the $E_i$ peak is finally defined by

$$F_c(E_i) = \frac{N(E_i)}{N^0(E_i)}. \quad (9)$$

Clearly sum peaks can be produced by any set of photons which can be emitted together, irrespective of the final level of a transition being the same as the initial level of the next transition or not and there being a single photon transition contributing to the same peak or not. The definitions in Eq. (5) are also valid in such cases, while the definitions of $U^{(n)}$ should be extended in an obvious way; under such circumstances, the count rate in the sum peak is given by a formula similar to Eq. (6). Also, in order to include these cases, we define $M^{(n)}$ as the set of all groups of n photons ($n = 1, 2, \ldots$) which can be emitted together in a decay process:

$$M^{(n)} = \{\{j_1, j_2 \ldots j_n\} \in T | p_{j_1,j_2 \ldots j_n} > 0\}, \quad (10)$$

where $M^{(n)} = T$ for $n = 1$; $U^{(n)}(i) \subset M^{(n)}$ for any $n$. Sets $S$ and $M$ are also related. As an example of this relationship, consider $\{j_1, j_2, \ldots, j_n\} \in S^{(n)}(q_1, q_2, \ldots, q_m)$; denote by $\{i_1, i_2, \ldots, i_{n+m}\}$ the set obtained by ordering $\{j_1, j_2, \ldots, j_n, q_1, q_2, \ldots, q_m\}$. According to the definition of $S^{(n)}$ we have $i_1, i_2, \ldots, i_{n+m} \in T$ and $p_{i_1,i_2,\ldots,i_{n+m}} > 0$. Consequently $\{i_1, i_2, \ldots, i_{n+m}\} \in M^{(n+m)}$. On the contrary, if from a set $\{i_1, i_2, \ldots, i_n\} \in M^{(n)}$ we extract a subset $\{q_1, q_2, \ldots, q_m\}$, the photons $\{j_1, j_2, \ldots, j_{n-m}\}$ which were not extracted represent a set included in $S^{(n-m)}(q_1, q_2, \ldots, q_m)$.

From the above discussion it is evident that for the evaluation of coincidence summing corrections it is necessary to provide procedures: (i) to compute the joint emission probability for any group of photons emitted by the nuclide; (ii) to identify all the groups of photons which belong to the sets of the type presented above; (iii) to evaluate the detection probability for the group of photons.

Items (i) and (ii) are presented below, while item (iii) can be found elsewhere (Sima et al., 2001; Sima and Arnold, 2000).

### 3.1. Preliminary step

The decay data required by GESPECOR are saved in a library called KORDATEN that is automatically compiled from the NUCLEIDE database (Bé et al., 2004) or from ENSDF. For each level $l$ several quantities are read from the KORDATEN library: the energy $E(l)$, the decay probability on that level $B(l)$, the $K$ and $L$ electron capture probability $P_K(l)$, $P_L(l)$ in the case of electron capture decay, and the level half life $\tau(l)$.

Consider each transition $i \in T$: levels $l$ and $m$ between which the transition takes place ($l = l_i(i)$ and $m = l_f(i)$, with $l,m \in L$, $l > m$), the photon energy $E_i$, the photon emission probability $p_i$, the total, the $K$ and $L$ conversion coefficients $\alpha(i)$, $\alpha_K(i)$ and $\alpha_L(i)$ are also read from KORDATEN. Then the total transition probability by photon emission and internal conversion, $p_t(l,m) = p_i[1+\alpha(i)]$, where $l = l_i(i)$ and $m = l_f(i)$ is calculated.

Next the transition probability $w_t(l,m)$ from level $l$ to level $m$ if the nucleus is already in the state $l$ is computed:

$$w_t(l,m) = \frac{p_t(l,m)}{\sum_{n=1}^{l-1} p_t(l,n)}. \tag{11}$$

The gamma emission probability of the $i$th transition between the states $l = l_i(i)$ and $m = l_f(i)$, if the nucleus is already in the initial state $l$ is given by the equation:

$$w(i) = w(l,m) = \frac{w_t(l,m)}{1+\alpha(i)}. \tag{12}$$

It is also useful to compute the transition probability $v(l,m)$ from level $l$ to level $m$ if the nucleus is already in the initial state $l$ by all possible sequences of transitions, i.e. by a direct transition $v_1(l,m)$, by a sequence of two linked transitions $v_2(l,m)$, by a sequence of three linked transitions $v_3(l,m)$ and so on up to the longest sequence, composed at most from $l$–$m$ transitions. The matrix $v(l,m)$ can be easily computed by simple recurrence relations, based on the following formulae:

$$v_1(l,m) = w_t(l,m), \tag{13a}$$

$$v_2(l,m) = \sum_{n=l-1}^{m+1} v_1(l,n) w_t(n,m), \tag{13b}$$

$$v_k(l,m) = \sum_{n=l-(k-1)}^{m+1} v_{k-1}(l,n) w_t(n,m), \quad k = 3,\ldots,(l-m). \tag{13c}$$

The above equations are the Chapman–Kolmogorov equations for the Markov chain with nuclear levels as states and $w_t$ as transition matrix between the states. It is easily seen that the matrix $v_k$ is equal to the $k$th power of matrix $w_t$ and consequently

$$v = w_t + (w_t)^2 + (w_t)^3 + \cdots + (w_t)^{l-m}. \tag{14}$$

The matrix $v$ is triangular, with 0 values on the diagonal.

The total feeding probability $F(l)$ of a level, both directly by the decay and by transitions from higher levels is determined by

$$F(l) = B(l) + \sum_{n=l+1}^{N} B(n) v(n,l). \tag{15}$$

### 3.2. Computation of the joint emission probability of groups of photons

Consider the group of photons emitted in the transitions $i_1, i_2, \ldots, i_m$, with $i_1 < i_2 < \ldots < i_m$. According to the rule for numbering the transitions, the group cannot be emitted in decay if there is a transition index $k = 1, 2, \ldots, m-1$ such that $l_f(i_k) < l_i(i_{k+1})$. The emission probability of the group of photons (irrespective of the fact that other photons are emitted or not in the same decay process) is:

$$\begin{aligned} p_{i_1,i_2,\ldots,i_m} = {} & F(l_i(i_1)) w(i_1)[\delta_{l_f(i_1),l_i(i_2)} + v(l_f(i_1), l_i(i_2))] \\ & \times w(i_2)[\delta_{l_f(i_2),l_i(i_3)} + v(l_f(i_2), l_i(i_3))] \ldots \\ & w(i_{m-1})[\delta_{l_f(i_{m-1}),l_i(i_m)} + v(l_f(i_{m-1}), l_i(i_m))] \\ & \times w(i_m)[\delta_{l_f(i_m),1} + v(l_f(i_m), 1)]. \end{aligned} \tag{16}$$

In the above equations we used the Kronecker symbol:

$$\delta_{i,j} = 1 \quad \text{if} \quad i = j, \tag{17a}$$

$$\delta_{i,j} = 0 \quad \text{if} \quad i \neq j. \tag{17b}$$

### 3.3. Selection of groups of photons

All possible groups of photons that can be emitted in the decay process can be easily enumerated for a nuclide with few levels. The task is much more difficult in the case of complex decay schemes: the abstract structure of the decay scheme should be considered in order to solve this problem in an efficient way, i.e. the abstract relation between the levels connected by transitions. Then the decay scheme can be represented by a graph and the methods developed in graph theory can be applied in defining the various sets of photons that can be emitted together in the decay process of the nucleus.

A graph is a mathematical object $G = \{V, E\}$ where $V = \{v_i\}$ is the set of vertices (or nodes) and $E = \{e_k\}$ is the set of edges (Bondy and Murty, 1982; Gross and Yellen, 2003). Each edge $e$ is represented by a pair of vertices; if $e = (u,v)$ where $e \in E$, $u,v \in V$, the vertices $u$ and $v$ are linked or related by the edge $e$. The existence of the edge $e = (u,v)$ means that there exists a relation between the vertices $u$ and $v$. Each edge can be represented by an ordered pair $(u,v)$ in a type of the graph which is called a directed graph or digraph; the pair $(u,v)$ represents an arc from $u$ to $v$ in a

digraph. Under these circumstances, if $e$ is an arc, $e=(u,v)\in E$, and as a result $u$ is in relation with $v$, but $v$ is not necessarily in relation with $u$. A walk in $G$ is defined as a sequence of vertices linked by edges (or by arcs in the case of a digraph). A walk in which no vertex is included more than once is called a trail; a trail in which no edge is included more than once is called a path in $G$. Finding walks, or trails or paths with specific properties are typical problems solved by graph theory.

The decay scheme of a nuclide can be represented by a digraph with $L$ as the set of vertices and $T$ as the set of arcs. Each level is considered a vertex, labeled by the level number. The transition from level $l$ to level $m$ is represented by an arc $(l,m)$ from vertex $l$ to vertex $m$. The arcs are labeled by the corresponding transition numbers. Any sequence of transitions in the decay process is represented by a path in the graph. The problem of finding the sets of photons emitted in a single decay act is equivalent to finding the paths in $G$ that satisfy specific conditions. We solved this problem by an algorithm of the breadth-first search type in which the $M^{(n)}$ sets are found consecutively in ascending order of $n$. Each valid set is consecutively numbered and the emission probability of the set is evaluated as presented in the previous section.

As an example of the algorithm we present the case of sets with three photons $M^{(3)}$. The set containing the transitions with the lowest numbers is clearly that composed from transition 1, then the first transition starting on the final level of transition 1 [this is the transition with number $t_i(l_f(1))$], followed by the first transition starting on the final level of this second transition; this set is $\{i_1^{(1)}, i_2^{(1)}, i_3^{(1)}\}$, with $i_1^{(1)}=1$, $i_2^{(1)}=t_i(l_f(i_1^{(1)}))$, $i_3^{(1)}=t_i(l_f(i_2^{(1)}))$, e.g. {1,5,8} in Fig. 1. The next set containing three photons is searched by replacing $i_3^{(1)}$ with the smallest $i_3^{(2)}>i_3^{(1)}$; set $\{i_1^{(1)}, i_2^{(1)}, i_3^{(2)}\}$ is a valid set if in the graph the initial vertex of $i_3^{(2)}$ is the same as the initial vertex of $i_3^{(1)}$ or if there is a path from the final vertex of $i_2^{(1)}$ to the initial vertex of $i_3^{(2)}$; the last condition is equivalent with $v(l_f(i_2^{(1)}), l_i(i_3^{(2)}))>0$; this is {1,5,11} in Fig. 1. The next set is searched by replacing $i_3^{(2)}$ with the smallest $i_3^{(3)}>i_3^{(2)}$ that satisfies the same conditions. The procedure is repeated until no additional set can be obtained by increasing the transition number of the third photon. Then backtracking is applied, i.e. the second photon $i_2^{(1)}$ is replaced by the smallest $i_2^{(2)}>i_2^{(1)}$ that either starts on the same level as $i_2^{(1)}$ or there is a path in the graph from the final level of transition $i_1^{(1)}$ to the initial level of transition $i_2^{(2)}$; the first trial for the third photon is $i_3^{(1)}=t_i(l_f(i_2^{(2)}))$, e.g. {1,6,9} in Fig. 1. Additional sets are found by replacing consecutively the third photon by photons emitted in higher number transitions ({1,6,10}, {1,6,11}) until all the possibilities are exhausted—the second photon from the set is then replaced {1,7,11} and the procedure is repeated until no additional set can be obtained (in Fig. 1 the last case possible is {1,9,11}). Backtracking is again applied, i.e. the first photon is replaced by a new photon with the smallest $i_1^{(2)}>i_1^{(1)}$, the second and third are re-initialized to $i_2^{(1)}=t_i(l_f(i_1^{(2)}))$, $i_3^{(1)}=t_i(l_f(i_2^{(1)}))$; this is the first set ({2,8,11}) with the new photon at the first position. The procedure is repeated until all the possibilities are exhausted. At this point all the $M^{(3)}$ sets have been discovered and the search for $M^{(4)}$ sets begins.

After the sets $M^{(n)}$ have been found, fast algorithms are applied for finding the $S^{(n)}$ and $U^{(m)}$ sets for the peaks of interest.

## 4. Formalism: the general case

When the nuclide has a metastable state $l$, after the total transition probabilities $w_t(l,m)$ were evaluated, the transition probabilities during the coincidence resolving time $\tau_C$ are computed:

$$w_C(l,m)=w_t(l,m)\{1-\exp[-\tau_C/\tau(l)]\}. \tag{18}$$

The photon emission probabilities from the same level are adjusted in a similar way. Also the Kronecker symbol in Eq. (16) is multiplied by $\{1-\exp[-\tau_C/\tau(l)]\}$. In all calculations of the joint emission probabilities $p_{i,j}$, $p_{i,j,k}$,… the quantity $w_t(l,m)$ is replaced by $w_C(l,m)$ and all $w(i)=w(l,m)$ are adjusted accordingly if $l$ is a metastable state.

Special procedures are implemented to deal with the X-rays and with the annihilation photons. More exactly, in the case of X-rays for each group of gamma photons besides the joint emission probability of the group, the emission probabilities of the group of gamma photons together with one X-ray, together with two X-rays, three X-rays and so on (up to 10 X-rays) are also evaluated. The sum of such probabilities is computed over the cases in which the photons can be emitted, e.g. the emission probability of the group of gamma photons together with X-rays emitted following electron capture decay (when appropriate) is added to the emission probability of the same group together with X-rays produced in any possible internal conversion transitions not corresponding to the gamma photons included in the group. For each group associated with $n$ X-rays, all the combinations of $n_\alpha$ $K_\alpha$ and $n_\beta$ $K_\beta$ X-rays ($n_\alpha+n_\beta=n$) are separately evaluated. Thus, the quantities $p_{i,j}(n_\alpha,n_\beta)$, $p_{i,j,k}(n_\alpha,n_\beta)$ and so on are computed.

Consider the case of annihilation photons: above each level $l$ fed by $\beta^+$ decay two levels are added in the first step with energies $E(l)+511$ and $E(l)+1022$ keV, where $E(l)$ is the energy of the level $l$. The transformed decay scheme is analyzed on the basis of the annihilation photons feeding different levels being different; so groups of photons that include annihilation quanta associated with different levels are considered as different and the probability of each group is evaluated separately. A second step involves the groups that differ only by the fact that the annihilation photons are associated with different levels being combined into a single equivalent group.

## 5. Conclusions

The tool implemented in GESPECOR to process decay scheme data and incorporate computation of coincidence summing corrections has been described. The main features of this tool are: (a) the possibility to analyze exactly decay schemes of arbitrary complexity, the only restriction being the study of nuclides with less than 100 levels; (b) the computation of the joint emission probability of any group of photons resulting from the decay (de-excitation gamma photons, $K_\alpha$ and $K_\beta$ photons from electron capture decay or from internal conversion and 511 keV annihilation photons from $\beta^+$ decay); (c) the possibility to read the decay data from the NUCLEIDE database (Bé et al., 2004) or from the ENSDF database. The output of this tool is ideal for providing the decay scheme data for the evaluation of coincidence summing corrections by Monte Carlo simulation methods.

## Acknowledgments

We would like to thank Dr. M.-M. Bé for providing the updated versions of NUCLEIDE database and software, and Drs. H. Janssen and E. Schönfeld for providing their tool for X-ray emission calculations.

## References

Andreev, D.S., Erokhina, K.I., Zvonov, V.S., Lemberg, I.Kh., 1972. Consideration of cascade transitions in determining the absolute yield of gamma rays. Instrum. Exp. Technol. 15, 1358 (English translation).

Arnold, D., Sima, O., 2001. Total versus effective total efficiency in the computation of coincidence summing corrections in gamma-ray spectrometry of volume sources. J. Radioanal. Nucl. Chem. 248 (2), 365–370.

Bé, M.-M., Browne, E., Chechev, V., Chisté, V., Dersch, R., Dulieu, C., Helmer, R.G., MacMahon, T.D., Nichols, A.L., Schönfeld, E., 2004. NUCLÉIDE, Table de radionucléide sur CD-ROM, Version 2-2004, CEA/BNM-LNHB, 91191, Gif-sur-Yvette, France.

Berlizov, A.N., Tryshyn, V.V., 2005. A Monte Carlo approach to true-coincidence summing correction factor calculation for gamma-ray spectrometry applications. J. Radioanal. Nucl. Chem. 264 (1), 169–174.

Bondy, J.A., Murty, U.S.R., 1982. Graph Theory with Applications, North-Holland, Amsterdam.

Debertin, K., Schötzig, U., 1979. Coincidence summing in Ge(Li) spectrometry at low source-to detector distance. Nucl. Instrum. Methods 158, 471–477.

ENSDF database, Evaluated Nuclear Structure Data File (ENSDF). Internet information at: ⟨http://ie.lbl.gov/databases/ensdfdata.exe⟩.

Gross, J.L., Yellen, J. (Eds.), 2003. Handbook of Graph Theory. CRC Press, Boca Raton.

Korun, M., Martinčič, R., 1993. Coincidence summing in gamma and X-ray spectrometry. Nucl. Instrum. Methods 325, 478–484.

Korun, M., Martinčič, R., 1995. Activity calculation for voluminous samples in the presence of coincidence summing effects. Nucl. Instrum. Methods 355, 600–608.

Laedermann, J.-P., Décombaz, M., 2000. Simulation of nuclear decay. Appl. Radiat. Isot. 52 (3), 419–425.

McCallum, G.J., Coote, G.E., 1975. Influence of source–detector distance on relative intensity and angular correlation measurements with Ge(Li) spectrometers. Nucl. Instrum. Methods 130, 189–197.

Semkow, T.M., Mehmood, G., Parekh, P.P., Virgil, M., 1990. Coincidence summing in gamma-ray spectroscopy. Nucl. Instrum. Methods 290, 437–444.

Sima, O., Arnold, D., 2000. Accurate computation of coincidence summing corrections in low level gamma-ray spectrometry. Appl. Radiat. Isot. 53 (1-2), 51–56.

Sima, O., Arnold, D., Dovlete, C., 2001. GESPECOR: a versatile tool in gamma-ray spectrometry. J. Radioanal. Nucl. Chem. 248 (2), 359–364.