Chapter 3

Cross-Section: Formulation and Uncertainty Analysis

A brief introduction to the formulation of the reaction cross-sections is provided along with the detailed discussion on the uncertainty analysis by using the ratio measurement technique. Section 3.1 of the present chapter is very general in nuclear reaction theory and can be found in any nuclear physics text book. The advantage of adding this section is to present a complete insight into the measurement and to provide a basic knowledge, which would be helpful to understand the following subsections 3.2.2 and 3.2.3.

3.1 Determination of the Reaction Cross-Section

The irradiation of a target with a beam of particles may lead to various reaction mechanisms among the projectile and target nuclei. As a result of these different interactions an equilibrated compound nucleus may be formed, which de-excites and produce many reaction residues by the emission of different particles like, γ, p, n, α etc. The residual nuclei thus formed are in their excited states. The excited residual nuclei may decay to lower states through their characteristic γ-ray emission. If ϕ is the flux of incident particle beam, N_0 is the initial number of nuclei present in the target and σ_r is the activation cross-section of the target nuclei through a particular reaction channel, then the final activation product may be given by,

$$N = N_0 \phi \sigma_r \tag{3.1}$$

The disintegration rate of the induced activity in the sample at a time t_c, after the end of irradiation can be given by the expression,

$$\left(\frac{dN}{dt}\right)_t = N \frac{[1 - exp(-\lambda t_i)]}{exp(\lambda t_c)} \tag{3.2}$$

where t_i is the time duration of irradiation of target, t_c is the cooling time and λ is the decay constant for the induced activity of the residual nuclei which is related to the half-life ($T_{1/2}$) by the expression,

$$\lambda = \frac{ln2}{T_{1/2}} \tag{3.3}$$

The factor $[1 - exp(-\lambda t_i)]$ is called the saturation correction. It should also be considered that the radioactive nuclei produced might have also decayed during the time of the irradiation process. Therefore, the number of radioactive nuclei decay in a very small time interval dt can be written as,

$$dN = N[1 - exp(-\lambda t_i)] exp(-\lambda t_c) dt \tag{3.4}$$

If the induced activity in the irradiated sample is recorded for a time $\triangle t$ after a lapse of time t_c, then the total number of nuclei decayed during the time t_c to $t_c + \triangle t$ is given by

$$C = \int_{t_c}^{t_c + \triangle t} dN \tag{3.5}$$

$$C = N[1 - exp(-\lambda t_i)] \int_{t_c}^{t_c + \triangle t} exp(-\lambda t_c) dt \tag{3.6}$$

$$C = N[1 - exp(-\lambda t_i)]\frac{[1 - exp(-\lambda \triangle t)]}{\lambda exp(\lambda t_c)} \tag{3.7}$$

$$C = N\frac{[1 - exp(-\lambda t_i)][1 - exp(-\lambda \triangle t)]}{\lambda exp(\lambda t_c)} \tag{3.8}$$

If the induced activity in the sample is recorded by a suitable γ-ray spectrometer having geometry dependent efficiency (ε_G), then absolute counting rate $'C'$ and the observed counting rate $'C_{obs}]'$ may be related as,

$$C = \frac{C_{obs}}{(\varepsilon_G)I_\gamma K} \tag{3.9}$$

where, T_γ is the branching ratio of the characteristic γ-ray [1], K is the correction factor for the self absorption γ-rays [2,3] in the target and can be given as,

$$K = \frac{[1 - exp(-\mu d)]}{\mu d} \tag{3.10}$$

where, μ is the γ-ray absorption coefficient for the target of thickness d.

Thus, the reaction cross-section σ_R of the evaporation residue at a given beam energy E can be written as,

$$\sigma_R = \frac{C_{obs}\lambda exp(\lambda t_c)}{N_0 \phi \varepsilon_G I_\gamma K[1 - exp(-\lambda t_i)][1 - exp(-\lambda \triangle t)]} \tag{3.11}$$

where, C_{obs} is the number of counts under the photo-peak of the characteristic γ-ray. The equation 3.11 can be used for the calculation of the reaction cross-section of a residue at a given energy. Since the counting time of the detector (T_R) and the actual time of counting (T_L) may differ due to the dead time of the detector, therefore, equation 3.11 may be modified as,

$$\boldsymbol{\sigma_R = \frac{C_{obs}\lambda(T_R/T_L)}{N_0 \phi \varepsilon_G I_\gamma K[1 - e^{-\lambda t_i}][e^{-\lambda t_c}][1 - e^{-\lambda T_L}]}} \tag{3.12}$$

where, C_{obs} is the observed counts for respective γ-ray from monitor reaction, T_R and T_L are the clock time and the live time for the counting of the spectrum, λ is the decay constant ($\lambda = 0.693/t_{1/2}$), I_γ is the branching ratio for the respective γ-ray taken from Ref. [1], N_0 is the total number of target nuclei in the sample and ϵ is the detector efficiency. A C++ program based on above formulation has been used for the calculation of measured cross-section using the counting statistics of the populated reaction residues. The residual nucleus of a particular reaction may, in general, emits γ-rays of more than one energy. In such cases, the cross-section for the same reaction can be determined separately from the observed intensities of different γ -rays originating from the same residue. The weighted average of the cross-sections from different γ-rays is taken as the final experimental value, which can be determined as follows,

If σ_1, σ_2, σ_3, ..., σ_n are the measured cross-section and $\triangle\sigma_1$, $\triangle\sigma_2$, $\triangle\sigma_3$,......, $\triangle\sigma_n$, are the respective experimental cross-sections for the same reaction due to different γ-rays, then $\sigma_1 \pm \triangle\sigma_1$, $\sigma_2 \pm \triangle\sigma_2$, $\sigma_3 \pm \triangle\sigma_3$,......, $\sigma_n \pm \triangle\sigma_n$ are the experimentally measured cross -section for a given reaction due to different γ-rays. Therefore, the weighted average cross-section ($\overline{\sigma}$) is determined as,

$$\overline{\sigma} = \frac{\sum w_i \sigma_i}{\sum w_i} \tag{3.13}$$

where,

$$w_i = \frac{1}{(\triangle\sigma_i)^2} \tag{3.14}$$

The internal error $I.E.$ is given by,

$$I.E. = \left[\sum w_i\right]^{-\frac{1}{2}} \tag{3.15}$$

Thus the $I.E.$ entirely depends on the individual observations.

However, the external error $E.E.$ is given by,

$$E.E. = \left[\frac{\sum w_i(\overline{\sigma_i} - \sigma_i)}{n(n-1)\sum w_i}\right]^{\frac{1}{2}} \tag{3.16}$$

Which depends on difference between observed and the mean value. Therefore, the internal error depends on the internal consistency , whereas the external error is a function of external consistency of the observations. These error calculations have also been incorporated in the computation of desired cross-sections at different γ energies.

The above formulation and the equations 3.12-3.16 can be directly used for the calculation of proton-induced reaction cross-sections as in the present work, the proton flux was measured using the Faraday cap or by monitoring the accelerator beam over the irradiation time. However, in case of the neutron-induced reactions the neutron flux can not be measured by any direct method, therefore, a monitor reaction was used in each case in order to determine the neutron flux by using the evaluated or experimental cross-sections as the primary input for the monitor reaction. Monitor reactions can also be used in proton-induced measurements, though, the method is useful for neutron-induced reactions where the accurate flux estimation is important. The neutron flux ($< \Phi >$) can be written as,

$$< \Phi >=< \sigma_W > \frac{C_{obs}\lambda(T_R/T_L)}{N_0\varepsilon_G I_\gamma K[1-exp(-\lambda t_i)]exp(-\lambda t_c)[1-exp(-\lambda T_L)]} \tag{3.17}$$

where, $< \sigma_W >$ is the flux weighted cross-section for the monitor reaction and rest of the quantities have their usual meanings for monitor reaction residue similar to the equation 3.12. The flux weighted cross-section $< \sigma_W >$ can be written in terms of the neutron flux ϕ_i and corresponding cross-section σ_i at an energy E_i can be written as,

$$< \sigma_W >= \frac{\int_{E_i} \phi_{E_i}\sigma_{E_i}}{\int_{E_i} \phi_{E_i}} \tag{3.18}$$

Therefore, the neutron-induced reaction cross-section σ_R can now be written with the help of equations 3.12 and 3.17 as,

$$\boldsymbol{\sigma_R = \frac{C_{obs}\lambda(T_R/T_L)}{N_0 < \Phi > \varepsilon_G I_\gamma K[1-e^{-\lambda t_i}][e^{-\lambda t_c}][1-e^{-\lambda T_L}]}} \tag{3.19}$$

The indirect calculation of neutron flux may lead to large uncertainties and strong correlations among the different quantities used in the measurement. Therefore, in case of neutron-induced reaction cross-section, the uncertainties in the measured data have been calculated using co-variance analysis [4,5], which has been widely used and recommended for the evaluation of uncertainties in the data. The details regarding the co-variance technique are given in the following section.

3.2 Uncertainty Propagation using Covariance Analysis

The covariance (correlation) analysis [5] is a mathematical tool based on the error estimation by predicting means and covariances in non-linear systems. The covariance analysis provides the best estimation of the uncertainty along with the cross-correlations among the measured quantities, which in this case, are the reaction cross-sections. Except the counting statistics from a spectrum, other quantities like, the γ-abundances, efficiency of detector, flux, half-life of residues, etc, are taken from different sources which probably contains significant errors. A review of the literature [6,7] for the reported uncertainties in the recently studied (n, γ) and (n, 2n) reaction cross-sections for ^{232}Th and ^{238}U isotopes and the most commonly

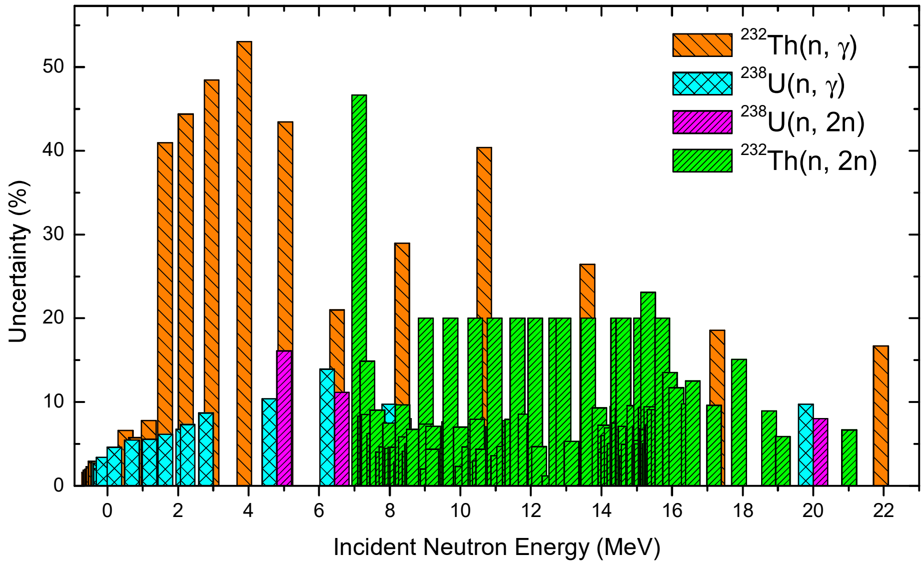

Figure 3.1: A pictorial representation of the uncertainties present in the (n, γ) and (n, 2n) reaction cross-sections of ^{232}Th and ^{238}U isotopes. The data were taken from the EXFOR [6] and ENDF/B-VII.1 [7] libraries.

used monitor reactions, listed in Table 2.4, show that, there is a minimum uncertainty of $\approx 5 - 10\%$ present only in the cross-sections used for the relative measurement of the nuclear data. A graphical representations are also shown in Figures 3.1 and 3.2. The uncertainties in the data presented in figure 3.1 were calculated by using quadratic sum of the statistical and systematic errors. In which the error from the monitor cross-sections were not included properly. It is obvious from the figure 3.2 that inclusion of the uncertainty from monitor cross-sections may further increase the total error present in the (n, γ) and (n, 2n) cross-sections. Here, covariance analysis plays a vital role as it transfers the errors from each quantity used in the calculations into the final uncertainties.

The method is based on the assumption that the result of an observation can be considered as a random variable $x = (x_1, x_2, x_3, ..., x_n)$. The normalization condition of the probability distribution $p(x)$ of x can be given as, $\int_{-\infty}^{+\infty} p(x)dx = 1$, where $dx = dx_1 dx_2 dx_3 ... dx_n$. The expectation value 'A' of a real-valued function $f(x)$ can be defined as,

$$A(f(x)) = \int_{-\infty}^{+\infty} f(x)p(x)dx \tag{3.20}$$

the mean and variance of variable x_k are given by,

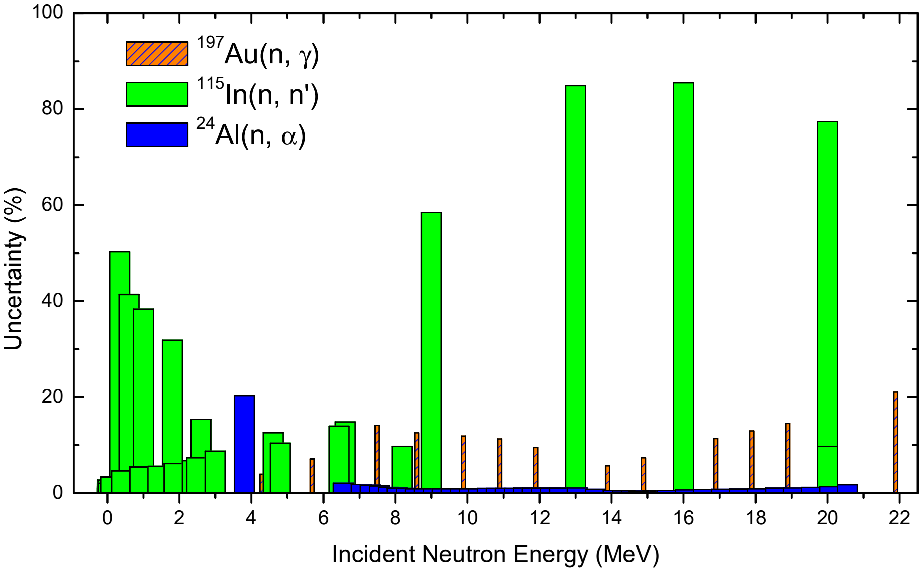

Figure 3.2: A pictorial representation of the uncertainties present in the commonly used monitor reactions. The data were taken from the EXFOR [6] and ENDF/B-VII.1 [7] libraries.

$$\tilde{\mathbf{x}}_{\mathbf{k}} = A(x_k); \quad \mathbf{Var}(x_k) = A[(x_k - \tilde{x}_k)^2] \tag{3.21}$$

Since, the variables are dependent, therefore, the covariance and the correlation among the variables x_k are defined as [5],

$$\mathbf{Cov}(x_k, x_i) = \int (x_k - \tilde{x}_k)(x_i - \tilde{x}_i)p(x_1, x_2 ... x_n)dx \tag{3.22}$$

$$\mathbf{Corr}(x_k, x_i) = \frac{Cov(x_k, x_i)}{\sqrt{Var(x_k)}\sqrt{Var(x_i)}} \tag{3.23}$$

where, $-1 \leq \mathbf{Corr}(x_k, x_i) \leq 1$ and the uncertainty can be defined as the standard deviation $\triangle x_k = \sqrt{\mathbf{Var}(x_k)}$.

3.2.1 Basic Concepts and Definitions

A number of input parameters (e.g., number of counts, number of incident particles, number of atoms in the sample) are used in the determination of reaction cross-section. we assign these parameters as random variables x_i (i=1,2,3,...) with a probability distribution function $p(x_1, x_2, ..)$ following a normalization condition $\int_{-\infty}^{+\infty} p(x_1, x_2, ..)dx = 1$, where $dx = dx_1 dx_2 ....$ The mean value of the function x_{im}, covariance $Cov(x_i, x_j)$, correlations

$Cor(x_i, x_j)$, variance $Var(x_i)$ and the standard deviation $\triangle x_i$ can be defined as,

$$x_{im} = \int x_i p(x_1, x_2, ..)dx \tag{3.24}$$

$$Cov(x_i, x_j) = \int (x_i - x_{im})(x_j - x_{im})p(x_1, x_2, ..)dx \tag{3.25}$$

$$Cor(x_i, x_j) = Cov(x_i, x_j)/\triangle x_i \triangle x_j; \tag{3.26}$$

$$0 \geq Cor(x_i, x_j) \leq 1; Cor(x_i, x_j) = 1(i = j)$$

$$Var(x_i) = \int (x_i - x_{im})^2 p(x_1, x_2, ..)dx = Cov(x_i, x_j) \tag{3.27}$$

$$\triangle x_i = \sqrt{Var(x_i)} \tag{3.28}$$

If a set of quantities say y_k are related to the parameter x_i by $y_k = y_k(x_1, x_2, ...)$, the relation can be linearized around the mean values as,

$$y_k = y_{km} + \sum_i a_{ki}(x_i - x_{im}) \tag{3.29}$$

where, $y_{km} = y_k(x_{1m}, x_{22m}, ...)$ and the sensitivity coefficient,

$$a_{ki} = (\partial y_k/\partial x_i)_{x_i = x_{im}}$$

The variance and covariance of y_k can be expressed in terms of x_i as,

$$Var(y_k) = Var\Big(\sum_i a_{ki}x_i\Big) = \sum_i a_{ki}^2 Var(x_i) + 2\sum_{i>j} Cov(x_i, x_j)a_{ij} \tag{3.30}$$

$$Cov(y_k, y_l) = Cov\Big(\sum_i a_{ki}x_i, \sum_j a_{lj}x_j\Big) = \sum_{i,j} a_{ki}Cov(x_i, x_j)a_{lj} \tag{3.31}$$

If the function y_k is expressed in the form of multiplication as,

$$y_k = \prod_i x_i^{g_{ki}}; \qquad g_{ki} = \pm 1, 0 \tag{3.32}$$

the sensitivity coefficient can now be modified as,

$$a_{ki} = g_{gki} y_{km}/x_{im} \tag{3.33}$$

If the parameters are uncorrelated then the equation 3.29 simplifies to,

$$(\triangle y_k/y_{km})^2 = \sum_i g_{ki}^2 (\triangle x_i/x_{im})^2 \tag{3.34}$$

If the correlation is present in parameters x_i, equations 3.29 and 3.30 are simplifies to,

$$(\triangle y_k/y_{km}) = \sum_i g_{ki}^2(\triangle x_i/x_{im}) + 2\sum_{i>j} Cov(x_i, x_j)g_{ij} \tag{3.35}$$

$$Cov(y_k, y_l) = \sum_{i,j} g_{ki}Cov(x_i, x_j)g_{lj} \tag{3.36}$$

When y_k can not be explained in terms of equation 3.31 and no correlation exists then the equations 3.29 and 3.30 can be written as,

$$(\triangle y_k/y_{km})^2 = \sum_i s_{ki}^2(\triangle x_i/x_{im})^2 \tag{3.37}$$

where $S_{ki} = (x_{im}/y_{km})a_{ki}$, is the relative sensitivity coefficient which gives the uncertainty in y_k due to the uncertainty in x_i.

When the two parameters, say x_1 & x_2, are equal and they are independent from rest of the set, then the probability distribution takes the form,

$$p(x_1, x_2, ...) = P(x_1)\delta(x_1 - x_2)Q(x_3, x_4, ...) \tag{3.38}$$

where $\delta(x)$ is the Dirac' delta function. By using the definition

$$\begin{aligned} \int dx_1 dx_2 P(x_1)\delta(x_1 - x_2)f(x_1, x_2) &= \int dx_1 P(x_1)f(x_1, x_1) \\ &= \int dx_2 P(x_2)f(x_2, x_2) \end{aligned} \tag{3.39}$$

for a given function $f(x_1, x_2)$, the variance and the covariance of x_1 and x_2 are related as,

$$Var(x_1) = Var(x_2) = Cov(x_1, x_2) \tag{3.40}$$

and hence $Cor(x_1, x_2) = 1$ (fully correlated). However, x_1 and x_2 are said to be uncorrelated, $Cor(x_1, x_2) = 0$, when x_1 and x_2 can be determined independently. A situation of partial correlation occurs when x_1 and x_2 are determined not independently, but still x_2 is not automatically determined from x_1 (e.g., two detection efficiencies obtained from the same efficiency curve characterized by parameters a, b,...). A general matrix representation for the fully correlated, uncorrelated, and partially correlated parameters x_1 and x_2 are shown below.

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} and \begin{bmatrix} 1 & q \\ q & 1 \end{bmatrix}; 0 < q < 1$$

Using the definitions given above, the covariance analysis can be performed to find the uncertainties and correlations among detector efficiencies at different γ-ray energies and reaction cross-sections at different incident neutron energies. A detailed discussion on both the calculations is provided in the following subsection.

3.2.2 Uncertainty in the Detector Efficiency

The geometry dependent efficiency of the HPGe detector is given by the relation,

$$\varepsilon = K_c \frac{C}{N_0 I_\gamma e^{-\lambda T} \bigtriangleup t} \tag{3.41}$$

where, N_0 is the disintegration rate of ^{152}Eu γ-ray source at the time of manufacturing, λ is the decay constant, T is the time interval between the date of manufacturing and the experiment, I_γ is the absolute intensity of the particular γ-ray and K_c are the correction factor for the coincidence-summing effect [8]. which were calculated using the EFFTRAN code [9].

The different sources of uncertainty in the measurement process which propagate as the uncertainty in the efficiency of the detector come from C, N_0, I_γ and $T_{1/2}$. Therefore, the efficiency of the detector can be written as the function of four attributes as,

$$\varepsilon = f(C, N_0, I_\gamma, T_{1/2}) \tag{3.42}$$

the standard deviation in efficiency can be given by the Taylor expansion of equation 3.42 as,

$$\bigtriangleup \varepsilon = (\frac{\partial \varepsilon}{\partial C}) \bigtriangleup C + (\frac{\partial \varepsilon}{\partial N_0}) \bigtriangleup N_o + (\frac{\partial \varepsilon}{\partial I_\gamma}) \bigtriangleup I_\gamma + (\frac{\partial \varepsilon}{\partial T_{1/2}}) \bigtriangleup T_{1/2} \tag{3.43}$$

now squaring both the sides of equation 3.43 and neglecting the higher order terms, we get,

$$\begin{aligned}
\sigma_\varepsilon^2 = {} & \Big(\frac{\partial \varepsilon}{\partial C}\Big)^2 \sigma_C^2 + \Big(\frac{\partial \varepsilon}{\partial N_0}\Big)^2 \sigma_{N_o}^2 + \Big(\frac{\partial \varepsilon}{\partial I_\gamma}\Big)^2 \sigma_{I_\gamma}^2 + \Big(\frac{\partial \varepsilon}{\partial T_{1/2}}\Big)^2 \sigma_{T_{1/2}}^2 + 2\Big(\frac{\partial \varepsilon}{\partial C}\Big)\Big(\frac{\partial \varepsilon}{\partial N_0}\Big)\sigma_{CN_0} \\
& + 2\Big(\frac{\partial \varepsilon}{\partial C}\Big)\Big(\frac{\partial \varepsilon}{\partial I_\gamma}\Big)\sigma_{CI_\gamma} + 2\Big(\frac{\partial \varepsilon}{\partial C}\Big)\Big(\frac{\partial \varepsilon}{\partial T_{1/2}}\Big)\sigma_{CT_{1/2}} + 2\Big(\frac{\partial \varepsilon}{\partial N_0}\Big)\Big(\frac{\partial \varepsilon}{\partial I_\gamma}\Big)\sigma_{N_oI_\gamma} \\
& + 2\Big(\frac{\partial \varepsilon}{\partial N_0}\Big)\Big(\frac{\partial \varepsilon}{\partial T_{1/2}}\Big)\sigma_{N_0T_{1/2}} + 2\Big(\frac{\partial \varepsilon}{\partial I_\gamma}\Big)\Big(\frac{\partial \varepsilon}{\partial T_{1/2}}\Big)\sigma_{I_\gamma T_{1/2}}
\end{aligned}$$

above equation states the law of error propagation in a single valued function and can be represented in a matrix notation as,

$$\sigma_\varepsilon^2 = \begin{bmatrix} \frac{\partial\varepsilon}{\partial C} & \frac{\partial\varepsilon}{\partial N_0} & \frac{\partial\varepsilon}{\partial I_\gamma} & \frac{\partial\varepsilon}{\partial T_{1/2}} \end{bmatrix} \begin{bmatrix} \sigma_C^2 & \sigma_{CN_0} & \sigma_{CI_\gamma} & \sigma_{CT_{1/2}} \\ \sigma_{CN_0} & \sigma_{N_0}^2 & \sigma_{N_0 I_\gamma} & \sigma_{N_0 T_{1/2}} \\ \sigma_{CI_\gamma} & \sigma_{N_0 I_\gamma} & \sigma_{I_\gamma}^2 & \sigma_{I_\gamma T_{1/2}} \\ \sigma_{CT_{1/2}} & \sigma_{N_0 T_{1/2}} & \sigma_{I_\gamma T_{1/2}} & \sigma_{T_{1/2}}^2 \end{bmatrix} \begin{bmatrix} \frac{\partial\varepsilon}{\partial C} \\ \frac{\partial\varepsilon}{\partial N_0} \\ \frac{\partial\varepsilon}{\partial I_\gamma} \\ \frac{\partial\varepsilon}{\partial T_{1/2}} \end{bmatrix} \tag{3.44}$$

The uncertainty in the detector efficiency due to the four attributes $(C, N_0, I_\gamma, T_{1/2})$ can be calculated using the quadratic sum formula for $'i'$ number of γ-lines as,

$$\sigma_\varepsilon^2 = \left(\frac{\partial\varepsilon}{\partial C}\right)^2 \sigma_C^2 + \left(\frac{\partial\varepsilon}{\partial N_0}\right)^2 \sigma_{N_o}^2 + \left(\frac{\partial\varepsilon}{\partial I_\gamma}\right)^2 \sigma_{I_\gamma}^2 + \left(\frac{\partial\varepsilon}{\partial T_{1/2}}\right)^2 \sigma_{T_{1/2}}^2 \tag{3.45}$$

which can be re-written as,

$$\left(\frac{\triangle\varepsilon_i}{\varepsilon_i}\right)^2 = \left(\frac{\triangle C_i}{C_i}\right)^2 + \left(\frac{\triangle N_o}{N_0}\right)^2 + \left(\frac{\triangle I_{\gamma_i}}{I_{\gamma_i}}\right)^2 + (t \triangle \lambda)^2 \tag{3.46}$$

where the uncertainty in decay constant is,

$$\triangle \lambda = \frac{0.693 T_{1/2}}{T_{1/2}^2} \tag{3.47}$$

Further the covariance matrix for 'i' number of measurements is given by the sandwich formula,

$$(V_\varepsilon)_{ij} = \sum_r e_{ir} S_{ijr} e_{jr} \tag{3.48}$$

where S_{ijr} is the micro–correlation between e_{ir} and e_{jr} due to the r^{th} attribute [10]. The micro-correlation between different attributes have been assigned on the assumptions [4,11] as follows,

- If the two quantities (say x_1, x_2) can be determined independently, then the correlation between them, $\mathbf{Corr}(x_1, x_2) = 0$ (uncorrelated), while $\mathbf{Corr}(x_1, x_2) = 1$ (fully correlated), when they are completely dependent. The situation $0 < \mathbf{Corr}(x_1, x_2) < 1$ occurs when x_1 and x_2 are determined not independently, but still x_2 is not automatically determined from x_1 [5].

- The Counts (C) of different γ-lines are uncorrelated as they were measured separately. Therefore, S_{ijr} for counts will be an identity matrix of order $i \times i$.

- The γ-abundance (I_γ) for different γ-lines of ^{152}Eu is a characteristic property of each γ-line and hence they are assigned as uncorrelated.

- Since, each γ-line will be following same half-life ($T_{1/2}$) during the nuclear decay, therefore, they are correlated. The S_{ijr} matrix in such case would be a square matrix of order $i \times i$ having all the elements as 1.

- The initial activity (N_0) will be common for each γ-line, therefore, it would be treated as correlated quantity.

depending upon the above discussion the S_{ijr} matrices for attributes C, N_0, I_γ and $T_{1/2}$ will be of the forms,

$$\begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} and \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix}$$

Since, the γ-rays taken into calculations (say E_i) may be different from those taken into account for efficiency calculations. Therefore, the detector efficiencies for the γ-lines $E_i$can be calculated using the interpolation model [4]

$$ln\varepsilon_i = \sum_m p_m (lnE_i)^{m-1} \tag{3.49}$$

where, p_m is the fitting parameter, m is the order of the model used for fitting and E_i are the energy of the γ-lines. The solution for equation (2.36) can be obtained by considering a linear model Z $= AP$, where, Z ($z_i = ln\varepsilon_i$) is a column matrix, A ($A_{im} = (lnE_i)^{m-1}$) is the design matrix with elements, and P is the matrix having parameters p_m, which can be estimated using the least square method. The covariance matrix for solution parameters is given by,

$$V_{\hat{p}} = (A' V_z^{-1} A)^{-1} \tag{3.50}$$

Now the values of parameters p_m can be calculated as,

$$\hat{P} = V_{\hat{p}} (A' V_z^{-1} Z) \tag{3.51}$$

where matrix V_z can be obtained by using the definition,

$$(V_z)_{ij} = \frac{(V_\epsilon)_{ij}}{< \epsilon_i >< \epsilon_j >} \tag{3.52}$$

The goodness of the fit can be calculated by,

$$\chi_m^2 = (Z - AP)' V_z^{-1} (Z - AP) \tag{3.53}$$

The fitting parameters can be obtained by using equation (2.38) with $V_{\hat{p}}$ as the covariance matrix for the γ-lines of energies E_i. The correlation matrix for E_i can easily be calculated using the covariance matrix $V_{\hat{p}}$ as,

$$\mathbf{Corr}(E_i, E_j) = \frac{\mathbf{Cov}(E_i, E_j)}{\sqrt{\mathbf{Var}(E_i)}\sqrt{\mathbf{Var}(E_j)}} \tag{3.54}$$

now the covariance matrix for the measured cross-sections can be calculated using the results of the calculations presented in this section.

The efficiencies for the γ-lines of the sample and monitor reactions can be calculated by using the fitting parameters into the equation 3.49. The covariance matrix then can be calculated by designing matrices Z and A for new efficiencies. and using the equations,

$$V_{z_{\epsilon_i}} = A' V_{\hat{p}} A \tag{3.55}$$

and

$$V_{\epsilon_{ij}} = \epsilon_i V_{z_{\epsilon_{ij}}} \epsilon_j \tag{3.56}$$

where, $V_{z_{\epsilon_i}}$ is the covariance matrix for the column matrix Z and $V_{\epsilon_{ij}}$ is the covariance matrix for the efficiencies of the sample and monitor reaction γ-lines.

3.2.3 Uncertainty in the Measurement of Reaction Cross-section

The ratio technique [5] has been used for the covariance analysis in activation cross-section measurements. We write equation 3.19 with the help of equation 3.17 as,

$$<\sigma_s> = <\sigma_m> \frac{C_s N_{0_m} \varepsilon_m I_{\gamma_m} f_{\lambda_m}}{C_m N_{0_s} \varepsilon_s I_{\gamma_s} f_{\lambda_s}} \tag{3.57}$$

with the time factor f defined as,

$$f = (1 - e^{-\lambda t_i})(e^{-\lambda t_c})(1 - e^{-\lambda T_L})/\lambda \tag{3.58}$$

where the sample reaction parameters are denoted with suffix 's' and the monitor reaction parameters with suffix 'm'. Following the definition presented in section 3.2.2, the uncertainty in measured cross-section can be given by the quadratic sum formula,

$$\Big(\frac{\triangle\sigma_r}{\sigma_r}\Big)^2 = \sum_a\Big(\frac{\triangle a_r}{a_r}\Big)^2 + \sum_a\Big(\frac{\triangle a_m}{a_m}\Big)^2 + \Big(\frac{\triangle\sigma_m}{\sigma_m}\Big)^2 \qquad (3.59)$$
$$a = a(C, N_0, \varepsilon, I_\gamma, f)$$

Since the decay constant λ is related to the cross-section through an exponential function, therefore, the uncertainty in the time factor should be propagated using the uncertainty in the decay constant by differentiating $'f'$ with respect to λ as,

$$\begin{aligned}\frac{\partial f}{\partial\lambda} = \frac{1}{\lambda^2}\Big[&\lambda\frac{d}{d\lambda}(1-e^{-\lambda t_i})(e^{-\lambda t_c})(1-e^{-\lambda T_L})\\ &-(1-e^{-\lambda t_i})(e^{-\lambda t_c})(1-e^{-\lambda T_L})\frac{d}{d\lambda}(\lambda)\Big]\end{aligned} \qquad (3.60)$$

now dividing equation3.60 by $(1-e^{-\lambda t_i})(e^{-\lambda t_c})(1-e^{-\lambda T_L})$, squaring and rearranging result in,

$$\frac{1}{f^2}\Big(\frac{\partial f}{\partial\lambda}\Big)^2 = \frac{1}{\lambda^2}\Big(\frac{\lambda t_i e^{-\lambda t_i}}{1-e^{-\lambda t_i}} - \lambda t_c + \frac{\lambda(T_L)e^{-\lambda(T_L)}}{1-e^{-\lambda(T_L)}} - 1\Big)^2 \qquad (3.61)$$

for λt_i, λt_c, and $\lambda LT \rightarrow 0$, the above equation can now be written as,

$$\Big(\frac{\triangle f}{f}\Big)^2 = s^2_{f\lambda}\Big(\frac{\triangle\lambda}{\lambda}\Big)^2 \qquad (3.62)$$

with the relative sensitivity given as,

$$s_{f\lambda} = \Big(\frac{\lambda t_i e^{-\lambda t_i}}{1-e^{-\lambda t_i}} - \lambda t_c + \frac{\lambda(T_L)e^{-\lambda(T_L)}}{1-e^{-\lambda(T_L)}} - 1\Big) \qquad (3.63)$$

Now the covariance matrix for the measured cross-sections can be calculated using the sandwich formula,

$$(V_\sigma)_{ij} = \sum_r e_{ir} S_{ijr} e_{jr} \qquad (3.64)$$

where S_{ijr} are the micro-correlation matrices for different attributes based on the discussion provided for equation (2.35). The correlation matrix can be calculated using (V_σ) by following equation (2.41) and the uncertainty in cross-section can be calculated as the square root of diagonal elements $((V_{\sigma_{ii}})^{1/2})$ of the covariance matrix. Detailed covariance analysis for typically measured $^{100}Mo(n,2n)^{99}Mo$ and $^{58}Ni(n,x)$ reactions are given in Appendix A.

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