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Theoretical Model Predictions for Production of Medically Used Radionuclides on Alpha Induced with Cobalt-59 At Energies of 25 - 172 MeV

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COMPLET code; Excitation function; Radionuclide production; Reaction cross section; TALYS-1.95 code

Research article

ABSTRACT

This study used the theoretical nuclear model codes COMPLET and TALYS-1.95 to make theoretical predictions of the medically important production cross-sections for Chromium-51, Manganese-54, Iron-59, Cobalt-59 and Cobalt-60 radionuclides produced in the interaction of alpha- projectile with Cobalt-59 target ≈ 25 – 172 MeV alpha-energies. The results were compared with the measured values in the EXFOR data library. Pearson's correlation coefficient indicates a strong and positive correlation between the predicted and the previously measured medically important production cross-sections for Chromium-51, Manganese-54, Iron-59, Cobalt-59, and Cobalt-60 radionuclides. Further, the results showed that except for Chromium-51, the COMPLET code predicts more successful outcomes than the TALYS-1.95.

INTRODUCTION

Nuclear reaction cross-section data are very important to the field of medical radiobiology in both diagnostic imaging and targeted therapy (Kebede, 2021), which is crucial for the optimized production of radionuclides. In nuclear medicine, radionuclides are used for various useful applications, such as diagnosis, therapy, prevention of many serious ailments, and research to evaluate metabolic, physiologic, and pathologic conditions of the human body (Aydin *et al*., 2007). The successful production and usage of these radionuclides extends to oncology, cardiology, and even psychiatry through imaging procedures where information about the function of every major organ and tissue of the human body can be generated. Many radionuclides used in nuclear medicine are produced in cyclotrons, accelerators, or nuclear reactors, and production is an important and constantly evolving issue. In addition to this, different radionuclides play significant roles in technological applications of importance to our daily lives and scientific research (Aydin *et al*., 2007; Kilinç *et al*.,2016).

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The Positron Emission Tomography (PET) imaging technique is widely used for planning, early diagnosis of cancer, and evaluation of the treatment response in patients with cancer. This imaging technique is also used to study diseases of the heart, brain, thyroid, etc. (Noori *et al.*, 2017) for example, Cobalt-57($T_{1/2}$ =272 d) is used as a marker to estimate organ size and for in vitro diagnostic kits. Similarly, Chromium-51 radionuclide ($T_{1/2}$=28 d) is used to label red blood cells and quantify gastro-intestinal protein loss (Aydin *et al.*, 2007; Kilinç *et al.*, 2016).

Production cross sections for charged particles, especially nuclear reactions on metals that are induced by alpha, are important in medical radioisotope production (Mohamed, 2006; Demir *et al.*, 2017). Accordingly, reasonable comparative theoretical reaction model studies with an experiment using light-charged projectiles (proton, deuteron, and alpha) are beneficial (Qaim *et al.*, 2016; Tárkányi *et al.*, 2019; Amanuel, 2023) because of the non-availability of experimental cross-section data for the production of medical radionuclides, particularly in alpha-induced reactions, which are limited and still need further investigations.

To optimize the production routes, charged particle-induced cross-sections are desired. To optimize the radioisotope produced, a full knowledge of the excitation function is necessary, which helps maximize the yield of the desired product and minimize the radioactive impurities (Qaim *et al.*, 2002).

In radionuclide production, accurate reaction cross-section data are required for well-controlled and maximized production routes (Mohamed, 2006; Qaim, 2010). Nuclear reaction model-based computer codes can be essential in predicting production cross-sections, particularly for radionuclides whose experimental data are either unavailable or have significant discrepancies. In addition, theoretical model predictions have played a crucial role in creating optimized reference cross-section data, particularly in producing medically useful radionuclides (Koning *et al.*, 2013) that were calculated using the Monte Carlo nuclear reaction simulation codes TALYS 1.95 and COMPLETE.

Despite all efforts, one of the crucial aspects of the reaction mechanisms study is finding optimized production routes for radionuclides, particularly for medically used radionuclides. Moreover, it is evident that the non-availability of experimental cross-section data for producing medically useful radionuclides, particularly in alpha-induced reaction, are very limited and need further investigation. Therefore, the present work focuses on finding optimized production routes for medically useful radionuclides produced in the reaction of α-projectile with ^{59}Co-target, more specifically, to evaluate the nuclear data for the production of Chromium-51, Manganese-54, Iron-59, Cobalt-59, and Cobalt-60 on alpha-induced Cobalt-59 at alpha energy of positron-emitting radionuclides.

MATERIALS AND METHODS

Several theoretical nuclear reaction model-based computer codes have been used to predict radionuclide production cross-sections (Koning *et al.*, 2013; Amanuel, 2023). In this work, predictions of production cross sections for ^{51}Cr, ^{54}Mn, ^{59}Fe, ^{and} ^{57,60}Co radionuclides produced in the interaction of alpha-projectile with Cobalt-59 target via (a, x) channel were carried out using the computer codes TALYS-

1.95 and COMPLETE. The results were compared with the experimental data (Michel *et al*., 1980).

These codes were prefered because they have been successful and widely used for predicting production cross-sections and evaluating reaction data (Amanuel, 2023). The present work also used the default values of the level density nuclear model TALYS-1.95 computer codes.

TALYS-1.95 Code

TALYS-1.95 code is an advanced version of the TALYS code family with additional features. TALYS was first developed in 1998, aiming to consolidate the understanding of nuclear reactions into a single software tool. This program integrates various models—including pre-equilibrium, direct, optical, statistical, and fission nuclear reaction models—enabling predictions across all open reaction channels within one calculation framework (Qaim *et al*., 2016). The Monte Carlo reaction code simulates various types of nuclear reactions, operating on a Linux system and written in FORTRAN. A significant advantage of employing a Monte Carlo method for nuclear data evaluation is its ability to extract a series of correlations from prior results. Consequently, the code was developed with the objective of delivering a comprehensive and accurate simulation of nuclear reactions involving neutrons, photons, protons, deuterons, tritons, ^{3}He, and alpha particles within the energy range of 1 keV to 200 MeV, with a few exceptions. The data generated or used by the code developed for the Monte Carlo method is derived from a reference input parameter library, combining reliable nuclear models with a focus on resilience and user-friendliness (Koning *et al*., 2013).

The theory of excitation functions for the generation of medical radioisotopes are obtained with alpha-induced reactions (a,x) for some radioisotopes used in clinical medicine that are relevant for the development of better nuclear reaction theory and for several medical applications were computed by using TALYS 1.95 code. In general, the reaction cross section for entrance channel α and exit channel β of this code can be expressed, using Hauser-Feshback (Hauser-Feshback, 1952) formalism as follows:

$$\sigma_{\alpha\beta} = \frac{\pi}{k^2} \sum_J \frac{(2J+1)}{(2i_\alpha+1)(2I_\alpha+1)} \frac{\sum_{s,\ell} T_\ell(\alpha) \sum_{s,'\ell'} T_{\ell'}(\beta)}{\sum_\alpha \sum_{s,\ell} T_\ell(\alpha)} \qquad (1)$$

Where s is the channel spin, T_ℓ represents the transmission coefficients, and l is the orbital angular momentum. The Hauser-Feshback formula is simplest for the energy-average angle integrated cross-section of statistical reactions (reaction cross-section leading to a single final state).

COMPLETE code

Computer code COMPLETE is a revised and improved version of the Alice code family with additional physics, corrections, and competencies and has been used to predict production cross-sections (Asres *et al*., 2018). This code has successfully predicted several nuclear data sets, particularly for the production of radionuclides used in nuclear medicine medical (Yiğit and Tel, 2013; Asres *et al*., 2019). This code utilizes the Weisskopf-Ewing (Weisskopf and Ewing, 1940) formulation for compound nucleus (CN) emission, along with Blann's hybrid and geometry-dependent hybrid models for particle emission (PE) (Blann and

Vonach, 1983). In the complete code, level densities of residual nuclei play a crucial role in deciding the shapes and absolute values of excitation functions (Akkoyun *et al.*, 2015). This code uses the Weisskopf-Ewing formulation to predict reaction cross-sections as follows:

$$\sigma_{\alpha\beta} d\varepsilon_{\beta} = \sigma_{CN}(\alpha) \frac{(2i_{\beta}+1) u_{\beta} \varepsilon_{\beta} \sigma_{CN}(\beta) \omega(u_{\beta}) du_{\beta}}{\sum_{\alpha} \int_{0}^{E_{\alpha}^{max}} (2i_{\alpha}+1) u_{\alpha} \varepsilon_{\alpha} \sigma_{CN}(\alpha) \omega(u_{\alpha}) du_{\alpha}} \quad (2)$$

Where u_{α} is the reduced mass of the ejectile α, and $\sigma_{CN}(\alpha)$ is the cross-section for the production of the CN.

Comparison between experimental and Theoretical results

As shown in figures 1–5, the theoretical and experimental reaction cross-sections are represented in relation to the projectile energies. Pearson's correlation coefficient quantifies the level of mutual statistical dependence between two variables (Baak *et al.*, 2020). Typically, their values range from -1 to +1 or 0 to +1, where 0 means no statistical association, +1 means the strongest possible association, and −1 means the strongest negative relation.

In general, the data of this study have been analyzed after the theoretical data have been generated using the computer codes TALYS-1.95 and COMPLETE. The theoretical and experimental total cross-section results are compared using Pearson's correlation coefficient. Correlation is a measure of association between two variables. The mathematical description is given by Tárkányi *et al.* (2019).

$$R = \frac{\sum_{i=1}^{N} (X_{T_i} - <X_T>)(X_{E_i} - <X_E>)}{(N-1)(S_{XT})(S_{XE})} \quad (3)$$

Where;

$$< X_T >= \frac{1}{N} \sum_{i}^{N} (X_{T_i}) \quad (4)$$

$$S_{XT} = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (X_{T_i} - < X_T >)} \quad (5)$$

$$< X_E >= \frac{1}{N} \sum_{i=1}^{N} (X_{E_i}) \quad (6)$$

$$S_{XE} = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (X_{E_i} - < X_E >)} \quad (7)$$

Where R is the correlation coefficient and unit less, $\langle X_T \rangle$ and $\langle X_E \rangle$ are the mean theoretical and experimental reaction cross-sections, respectively, X_{T_i} and X_{E_i} are the theoretical and experimental total cross-sections of the ith value, respectively, whereas N is the number of the theoretical and experimental data, and S_{XE} and S_{XT} are the standard deviations of the experimental and theoretical total cross-sections, respectively. If $0 \leq R \leq 0.3$, the correlation is weak and positive, $0.3 \leq R \leq 0.7$ describes a moderate correlation, and $0.7 \leq R \leq 1$, the correlation is strong (Baak *et al.*, 2020).

RESULTS AND DISCUSSION

The current work investigated the excitation functions of medically important Chromium-51, Mangenes-54, Iron-59, Cobalt-59, and Cobalt-60 radionuclides produced in the interaction of alpha-projectile with Cobalt-59 target at 25–172 MeV alpha-energies. In addition, the experimentally measured excitation functions available in the literature (Michel *et al.*, 1980) were compared using the nuclear reaction-model codes TALYS-1.95 and COMPLET.

In COMPLETE code, the level density parameter a, which predominantly influence the equilibrium state components of a cross-section, is computed from the expression:

$$a = \frac{A_{CN}}{K} \quad (8)$$

Where A is the nucleon number of a compound system, and K is an adjustable constant, which may be varied to match the experimental data. For the present system, a representative ^{59}Co (α, x) ^{60}Co reaction, the value of K was varied (K = values of 8, 10, and 12 were used) to match the experimental data. A value of K = 10 in general reproduced satisfactorily experimentally measured EFs for Cobalt-60 residue. This value is consistently used for other residues populated in the interaction of the alpha-projectile with the target Cobalt-59. For the same representative Cobelt-60 residue, the initial exciton numbers n_o = 4 (2,2,0), 5 (2,2,1) were varied, and it was found that a value of n_o = 4 (2,2,0) better reproduced the measured excitation function (Michel and Brinkmann, 1980). For COMPLETE code prediction, K = 10 and n_o = 4 are consistently used for all residues populated in the interaction of the alpha-projectile with the target Cobalt-59.

Production of Chromium-51 radionuclide

Figure 1 illustrates the excitation functions for the Chromium-51 radionuclide, which were predicted theoretically and measured experimentally, as produced through the (α, x) channel during the interaction of the alpha projectile with the Cobalt-59 target. By using the TALYS-1.95 code, predicted cross-section values, except at alpha energies of 90–120 MeV, are in very good agreement with the measurements of Michel and Brinkmann (1980). It may further be seen that COMPLETE code predicted cross-section values that were generally in satisfactory agreement with the measured values of Michel and Brinkmann (1980).

Table 1 reveals that the Pearson's correlation coefficient values for the cross-section predictions from TALYS-1.95 and the COMPLETE code indicate a strong positive correlation between the theoretically predicted and experimentally measured production cross-sections (Michel and Brinkmann, 1980).

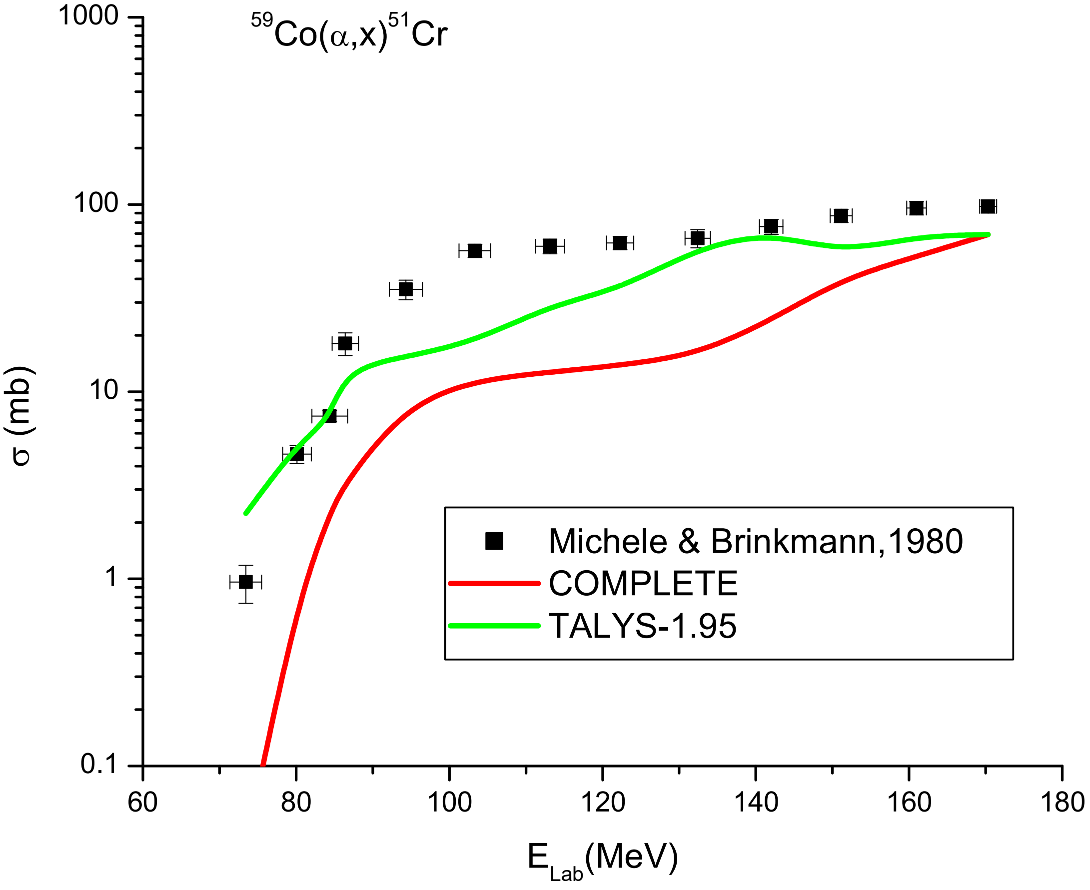

Figure 1. The experimentally measured and theoretically predicted excitation functions for medically used Crominum-51.

Production of Manganese-54 Radionuclide

The experimentally quantified production cross-sections for Manganese-54 radionuclide from the existing literature are compared with the theoretical predictions obtained using the COMPLET and TALYS-1.95 codes. Figure 2 shows the quantified excitation functions along with theoretical predictions for Manganese-54 radionuclide produced through the (α, x) channel in the interaction of alpha-projectile with a Cobalt-59 target at 25 MeV–172 MeV. Using COMPLETE code, predicted cross-section values except for 60 MeV–90 MeV are in very good agreement with the cross-section values measured by Michel and Brinkmann (1980). Figure 2 shows that the predicted cross-section values using the TALYS-1.95 code generally minimize the measured values of Michel and Brinkmann (1980). The COMPLETE code predicted production cross sections for Manigenes-54 radionuclide to have a peak value of 111 mb at ≈170 MeV.

Furthermore, it may be observed from Table 1 that, for Manganese-54 radionuclide, Pearson's correlation coefficient values between theoretically anticipated on COMPLETE and experimentally quantified production cross sections confirmed moderately positive correlations. In contrast, Pearson's correlation coefficient values between theoretically predicted using TALYS-1.95 and experimentally quantified production cross-sections confirmed strong positive correlations.

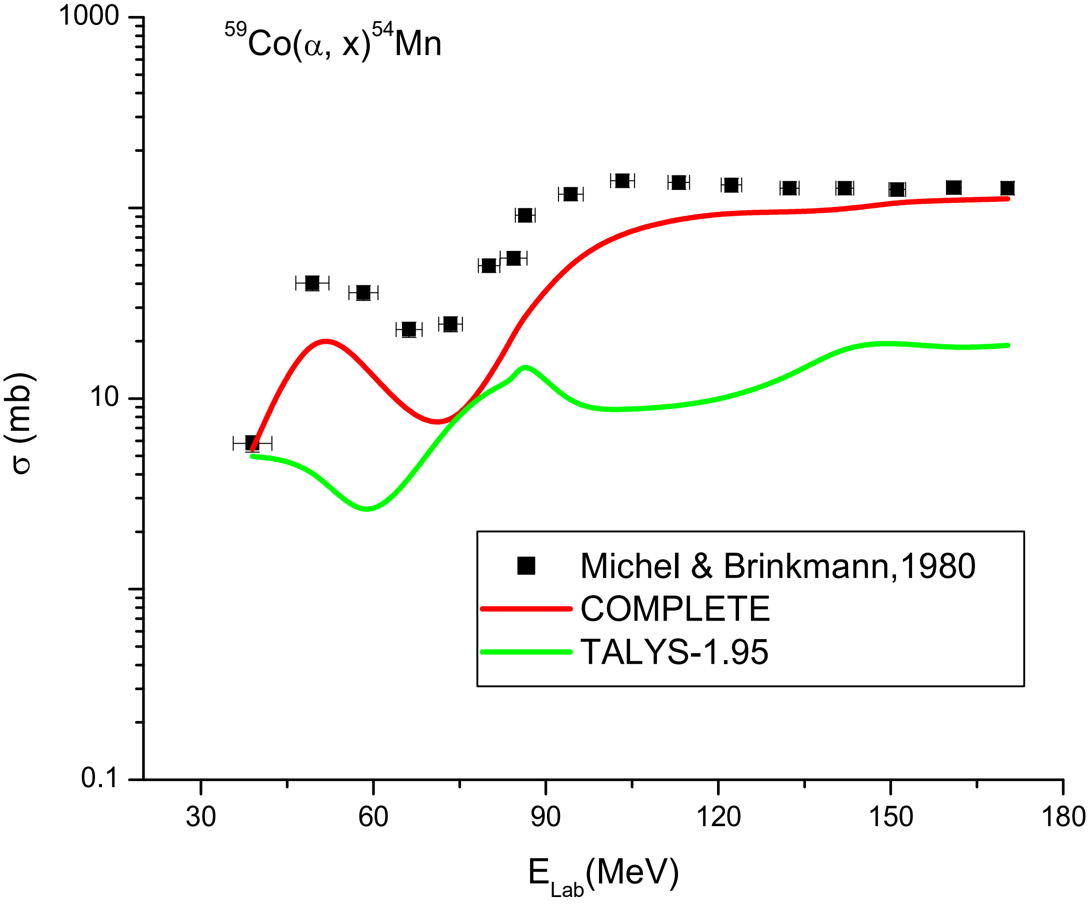

Figure 2. The experimentally measured and theoretically predicted excitation functions for medically used Manganese-54.

Production of Iron-59 radionuclide

Figure 3 shows the experimentally quantified excitation functions along with theoretical predictions obtained using TALYS-1.95 and COMPLETE codes for Iron-59 radionuclide produced via (α, x) channel in the interaction of alpha-projectile with the Cobalt-59 target. Using COMPLETE code, the predicted cross-section values in the energy range 55–172 MeV usually agree with the experimental measurements of Michel and Brinkmann (1980). However, the prediction of COMPLETE code below 55 MeV underestimates the cross-section values measured by Michel and Brinkmann (1980). It may further be observed from Figure 3 that the predicted cross-section values at low energy using the TALYS-1.95 code are in satisfactory agreement with the measured cross-section values of Michel and Brinkmann (1980). On the contrary, the predicted cross-section values at a high energy range using the TALYS-1.95 code underestimate the measured cross-section values of Michel and Brinkmann (1980).

Moreover, Table 1 further reveals that the Pearson's correlation coefficient values for the Iron-59 radionuclide indicate strong positive correlations between the cross-section values predicted by the COMPLETE code and those measured by Michel and Brinkmann (1980).

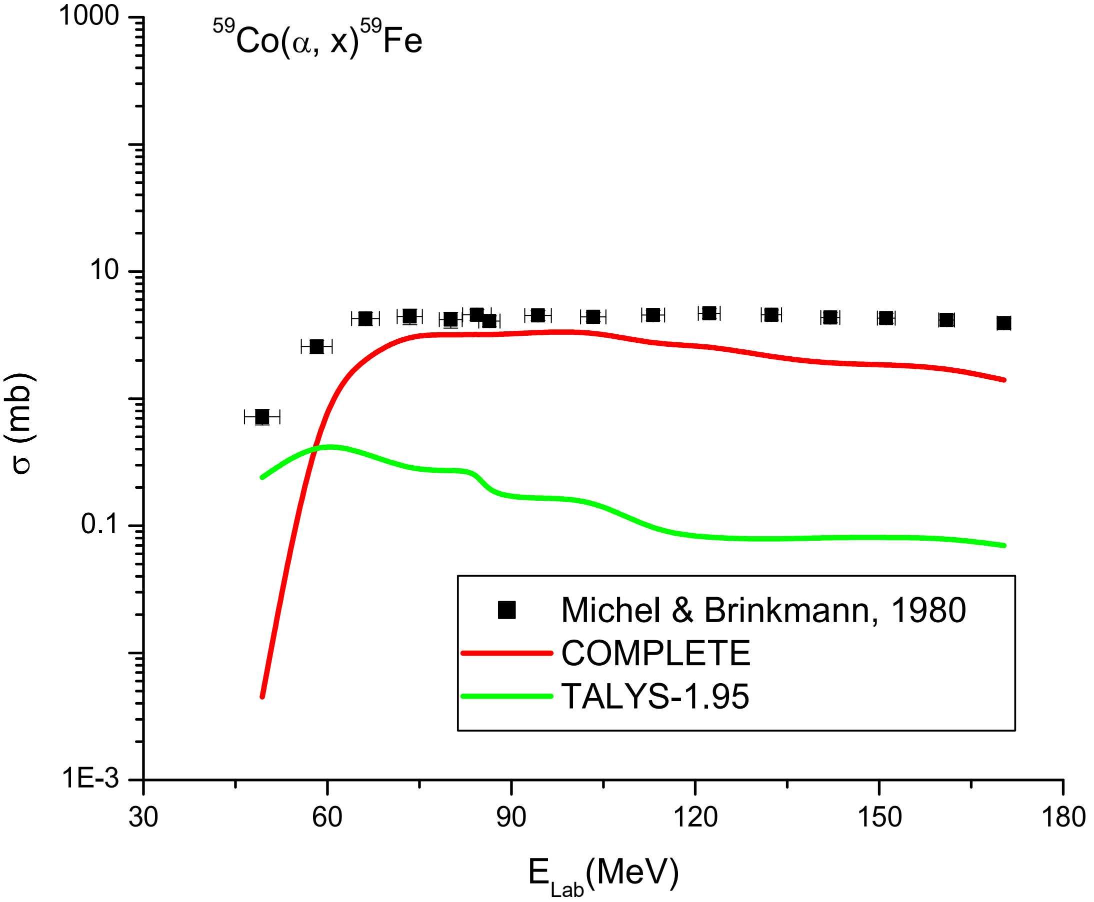

Figure 3. The experimentally measured and theoretically predicted excitation functions for medically used Iron-59.

Production of Cobalt-57 radionuclide

In Figure 4, the measured excitation functions for the medically used Cobalt-57 radionuclide produced via the complex (α, x) channel in the interaction of alpha-projectile with Cobalt-59 target are clearly presented along with the theoretically predicted excitation functions by using the TALYS-1.95 and COMPLETE codes. Using COMPLETE code, predicted production cross-sections are in very good agreement with the measured values of Michel and Brinkmann (1980). Using the TALYS-1.95 code, predicted production cross sections in the energy range 30 MeV–90 MeV are in very good agreement with the measured values (Michel and Brinkmann, 1980). However, predicted production cross sections using the TALYS-1.95 code at energies above 90 MeV are in satisfactory agreement with the measured values of Michel and Brinkmann (1980). The COMPLETE predicted production cross sections for Cobalt-57 radionuclide have a maximum value of ≈207 mb at ≈39 MeV. Furthermore, Table 1 clearly shows and confirmed that Pearson's correlation coefficient values for Cobalt-57 radionuclide has strong and positive correlations between the cross-section values predicted and the values measured by Michel and Brinkmann (1980).

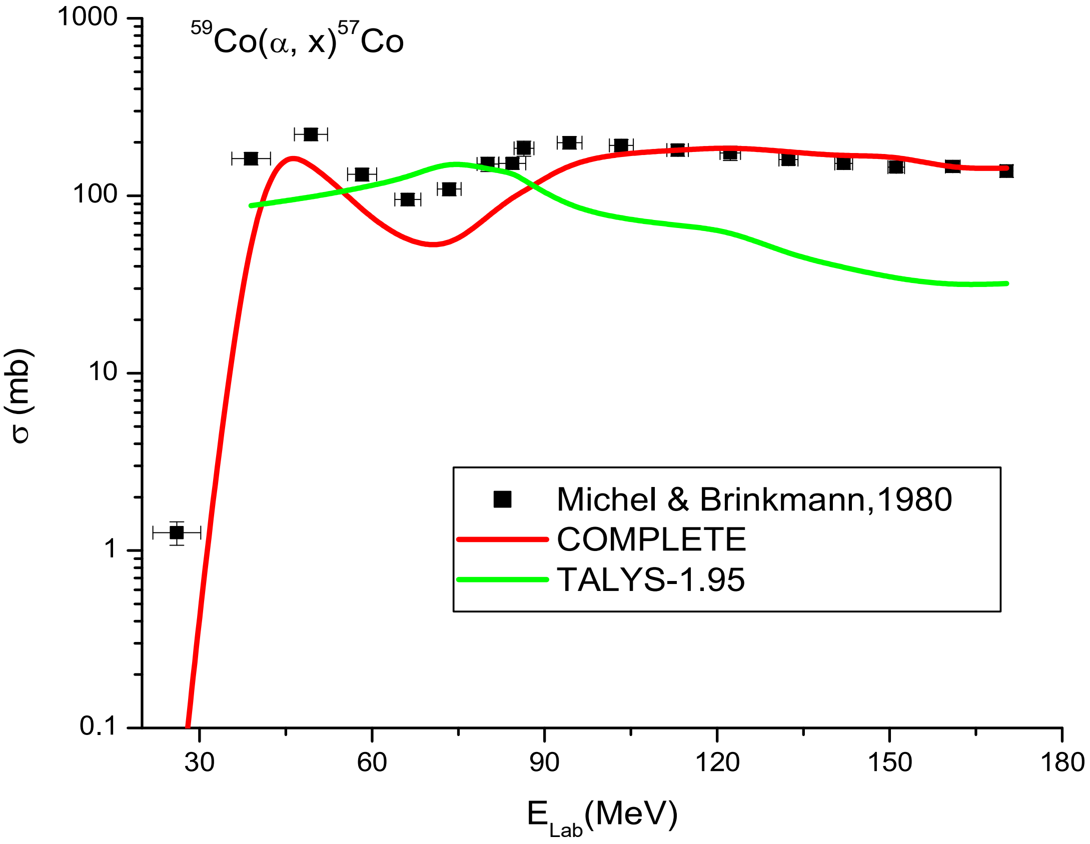

Figure 4. The experimentally measured and theoretically predicted excitation functions for medically used Cobalt-57

Production of Cobalt-60 Radionuclide

Figure 5 displays the experimentally quantified and theoretically predicted excitation functions for the medically used Cobalt-60 radionuclide produced in alpha-projectile interaction with the Cobalt-59 target via complex (α, x) channel. The cross-section values predicted using COMPLETE codes usually exaggerate the cross-section values measured by Michel and

Brinkmann (1980). However, predicted production cross sections in the energy range 30 MeV – 45 MeV are in very good agreement with the measured values of Michel and Brinkmann (1980). The prediction of the TALYS-1.95 code underestimates the cross-section values of the measurement of Michel and Brinkmann (1980). Moreover, the attainable value of the production cross section for Cobalt-60 radionuclide obtained using the COMPLETE code is about ≈343 mb at ≈39 MeV. The result on Table 1 further revealed that Pearson's correlation coefficient values between theoretically predicted, and experimentally quantified production cross-sections confirmed strong and positive associations.

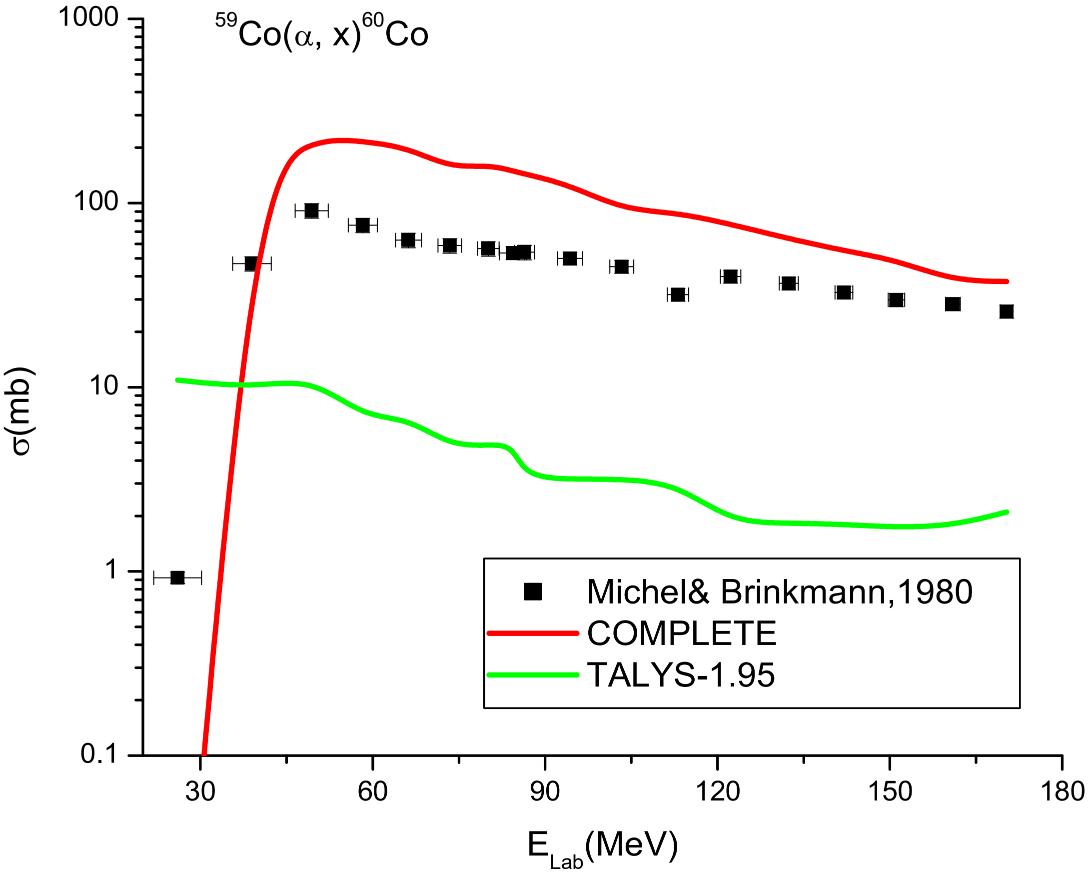

Figure 5. The experimentally measured and theoretically predicted excitation functions for medically used Cobalt-60.

Table 1. Pearson's correlation coefficient, R, between experimental measurements by Michel and Brinkmann (1980) and theoretical predictions

Radionuclide	TALYS-1.95 [COMPLETE]
^{51}Cr	0.921 [0.86]
^{54}Mn	0.65 [0.92]
^{59}Fe	- [0.84]
^{57}Co	0.5 [0.76]
^{60}Co	0.4 [0.96]

CONCLUSION

Excitation functions for the production of radionuclides from the alpha-bombardment of Cobalt-59 were studied for alpha-energies from 25 to 172.5 MeV. The theoretical nuclear reaction model codes COMPLET and TALYS-1.95 were used to logically predict the medically important production cross-sections for Chromium-51, Mangenes-54, Iron-59, Cobalt-59, and Cobalt-60 radionuclides produced in the interaction of alpha-projectile with Cobalt-59 target ≈ 25 - 172 MeV alpha-energies. The results were compared with the measured values in the EXFOR data library. Pearson's correlation coefficient shows a robust positive relationship between the predicted and previously observed production cross-sections for the medically relevant radionuclides Chromium-51, Iron-59, Manganese-54, Cobalt-59, and Cobalt-60. Further, the results show that except for Chromium-51, the COMPLETE code predicts more successful outcomes than the TALYS-1.95.

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