PAPER

The study of alpha particle induced reactions on bismuth-209 isotopes using computer code COMPLET

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Abstract

Calculations of the excitation function of ⁰⁹⁰⁹Bi (α, n)⁰⁲¹₂At, ⁰⁹⁰⁹Bi (α, 2n)⁰¹¹¹At and ⁰⁹⁰⁹Bi (α, 3n)⁰²¹⁰At reactions have been focussed on alpha induced reaction. Energy ranges of alpha particles were taken into computations as 10 MeV to 70 MeV. The objective of this study is to compare the computed results with the experimental data existing in the literature for each reactions. The calculated ⁰⁹⁰⁹Bi(α,xn) reaction cross-sections were computed using computer code COMPLET and were then compared with the experimental nuclear reaction data obtained from EXFOR library in the literature. This calculated data was analyzed and interpreted with tabular and graphical descriptions. Good agreement was found between the experimental and theoretical data. The results were briefly discussed within the text of this research work.

1. Introduction

Nuclear reaction is said to occur when a nuclear particle comes into close contact with another particle. During interaction, an exchange of energy and momentum are characterized by the incoming nuclei and the outgoing reaction products [1, 2]. Studying nuclear reaction leads to several fundamental discoveries and an understanding of the mechanism for the production of a new state of matter [3, 4]. The reaction mechanism is considered to proceed through equilibrium (EQ) as well as pre-equilibrium (PE) emission of particles of moderate excitation energies [2].

Theoretical calculations on the production cross-section of radioisotopes have an undeniable importance for the investigation of the new production routes as it can be seen from the many studies in the literature [5, 6]. Results from cross-section calculations have been compared with the experimental data taken from the EXFOR database [7].

Although the excitation function for Bismuth-209 was measured earlier by few groups, their research results differ to a large extent, hence precise and accurate measurements are still needed [8, 9]. A lot of work has been done on the study of excitation function of alpha-induced reactions for various target nuclei over a wide range of energy. The comparisons between theory and experiment of ⁰⁹⁰⁹Bi-isotopes have not been studied well [5, 10]. A theoretical analysis of the data has been carried out under the calculations based on hybrid and geometry dependent hybrid models using the computer code COMPLET which contains both compound and PE processes [9, 10]. With this motivation the present work was undertaken to calculate the excitation function for ⁰⁹⁰⁹Bi with 10 MeV to 70 MeV alpha-particle energy and compare the computed results with the experimental data existing in the literature for each reactions.

In this research work, the reaction cross-sections have been calculated for ⁰⁹⁰⁹Bi (α, n)⁰²¹₂At, ⁰⁹⁰⁹Bi (α, 2n)⁰¹¹¹At and ⁰⁹⁰⁹Bi (α, 3n)⁰²¹⁰At using computer code COMPLET and EXFOR data centre [6, 11]. Considering the importance of the best level density parameters and exciton numbers that influence the calculation of cross-section, the outputs of calculated results have been analysed and compared with the experimental data taken from EXFOR database [12].

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In our previous paper we discussed fission reaction of the target uranium isotopes for the given parameter of neutron-neutron converter [2]. This paper addressed the problem of evaluating the significance/correlation on the underlying theory and experimental aspects of nuclear physics inorder to find answers to the unanswered questions for the 21st century.

2. Methodologies

2.1. EXFORE data center
EXFOR is the ‘ExchangeFormat’ for the formation of experimental reaction data between national and international nuclear data centers [13]. The EXFOR (ExchangeFormat) format was designed for the collection, exchange and dissemination of microscopic neutron-induced reaction data based on a combination of keywords, coded information and free text [14–16]. The EXFOR format was further developed to cover charged-particle induced and photo-nuclear reaction data in addition to neutron-induced reaction data. The format is flexible in order to record all the necessary information to explain the measured data, but it also defines computer readable coded information [17, 18]. It is used for the benefits of researchers, scholars and nuclear users in all countries. It is the library and format for the collection, storage, exchange and retrieval of experimental nuclear reaction data. Although the EXFOR format can be used for both compilation and dissemination, centres may have their own formats for data services.

EXFOR is derived from ‘ExchangeFormat’ experimental nuclear reaction data compiled regularly through the network of nuclear reaction data centers [14, 19].

2.2. Computer code COMPLET
Various computer codes were developed based on different nuclear models which are enable to study nuclear structure and reaction mechanisms. The computer code COMPLET is an improved version of ALICE-91 [20]. This code is capable of calculating equilibrium and pre-equilibrium reaction cross-sections. This computer code system is used for the analysis and prediction of nuclear reactions and helped us to determine both the compound and pre compound excitation functions [17]. This code has been instrumental in producing numerous nuclear data evaluations. The structure of the code has become very complicated and somewhat cumbersome to upgrade or even simply maintain [2]. The advent of the modern FORTRAN (Formula-Translation) 90/95 scientific language has open the path toward modern and higher-level programing techniques that can be implemented efficiently to create a modern and powerful version of the computer code COMPLET [20]. Infact, the COMPLET computer code is really a collection of such FORTRAN modules, each dealing with a specific part of the nuclear reaction sequence calculations [7].

Excitation function is a function of energy and the theoretical results are compared with the experimental data obtained from EXFOR database [18, 21].

The nuclear level density parameters which are very essential quantity, influence the shape and the height of the calculated excitation functions [10]. The default value for the level density parameter and exciton number is taken to be taken as (8, 9, 10) and (4, 5 and 6) respectively [17, 22].

The theoretical and experimental reaction cross-sections results of bismuth–209 induced by alpha particle using computer code COMPLET as seen in (figures 1 to 3 and tables 1 to 3) are compared using scientific research method [10, 21]. The best level density parameter has been choosen for each reaction and radioisotope activities.

Figure 1. Comparison between theory and experiment of $^{209}$Bi ($\alpha$, n)$^{212}$At reaction cross-section.
Table 1. Results from the computer code COMPLET evaluation of $^{209}$Bi$(\alpha, n)^{212}$At reaction cross section compared with experimental data [23].

| Energy (MeV) | Experimental | Pre compound (theo) | Compound (theo) |
|-------------|--------------|---------------------|-----------------|
| 16.00       | 0.039        | 0.333 ± 0.000       | 0.333 ± 0.0     |
| 16.25       | 0.066        | 0.498 ± 0.000       | 0.498 ± 0.0     |
| 16.50       | 0.121        | 0.737 ± 0.000       | 0.737 ± 0.0     |
| 17.00       | 0.295        | 1.57 ± 0.799        | 1.57 ± 0.799    |
| 17.50       | 0.740        | 3.21 ± 0.559        | 3.21 ± 0.559    |
| 18.00       | 3.580        | 6.33 ± 0.397        | 6.33 ± 0.397    |
| 18.75       | 5.430        | 16.4 ± 0.247        | 16.4 ± 0.247    |
| 19.00       | 7.550        | 22.1 ± 0.213        | 22.1 ± 0.213    |
| 19.25       | 11.29        | 29.4 ± 0.184        | 29.4 ± 0.184    |
| 19.50       | 15.60        | 38.7 ± 0.161        | 38.7 ± 0.161    |
| 19.75       | 21.80        | 45.7 ± 0.148        | 45.6 ± 0.148    |
| 20.00       | 27.50        | 55.6 ± 0.134        | 55.5 ± 0.134    |
| 20.25       | 37.90        | 69.9 ± 0.120        | 69.8 ± 0.120    |
| 20.50       | 49.40        | 84.2 ± 0.109        | 84.1 ± 0.109    |
| 20.75       | 57.30        | 74.4 ± 0.116        | 74.2 ± 0.116    |
| 21.00       | 66.80        | 77.8 ± 0.113        | 77.5 ± 0.114    |
| 21.25       | 47.80        | 85.3 ± 0.108        | 84.7 ± 0.109    |
| 21.50       | 78.60        | 90.9 ± 0.105        | 90.1 ± 0.105    |
| 22.00       | 75.50        | 66.8 ± 0.122        | 65.6 ± 0.123    |
| 22.50       | 65.10        | 73.9 ± 0.116        | 72.1 ± 0.118    |
| 23.00       | 52.00        | 52.7 ± 0.138        | 50.5 ± 0.141    |
| 23.50       | 39.00        | 41.4 ± 0.155        | 38.5 ± 0.161    |
| 24.00       | 38.20        | 27.9 ± 0.189        | 25.0 ± 0.200    |

2.3. Computer code COMPLET calculations

Computer code COMPLET employed Weisskopf-Ewing model for the statistical component and Hybrid as well as geometry dependent hybrid model of Blann for PE emission [8, 21].

Many experimental methods have been developed to evaluate the reaction cross-section of various nuclear reactions. The nuclear reaction cross-section data are significant for several technical applications such as medical radionuclide production, accelerator-driven system, fission, fusion, dosometry, radiation therapy etc [20]. The calculated data has been compared with available experimental cross-sections data and theoretical data which is latest theoretical data for use in nuclear science and technology applications.

The calculated $(\alpha, n)$ and $(\alpha, 2n)$ $(\alpha, 3n)$ reaction cross sections for $^{209}$Bi$(\alpha, n)^{212}$At, $^{209}$Bi$(\alpha, 2n)^{211}$At and $^{209}$Bi$(\alpha, 3n)^{210}$At are shown in figures 3.1 to 3.4 [1]. The obtained results were then compared with the experimental data existing in the EXFOR databases [24, 25]. The values of the cross section were expressed in $(10^{-3}$ barns), while that of energies in (MeV) [15].

The data is collected using computer code COMPLET, from the experimental Data Center (EXFOR, IAEA) [14, 18]. These organized data are described graphically with the help of spreadsheet, analysed and interpreted accordingly and compared with the experimental data [2, 14].

The level density parameter influences the shape as well as the height of the calculated excitation functions. The level density parameter $a = \Lambda/\bar{a}$ was used for all nuclei, where $\Lambda$ is the mass number of the nucleus [2].

2.4. Comparisons between experimental and theoretical results

The general characteristics and procedures for irradiation, activity assessment and data evaluation (including estimation of uncertainties) were similar as in many of our earlier works. The correlation between the theoretical and experimental total cross-section results were evaluated using Pearson’s correlation coefficient ($R$) [2]:

$$R = \frac{\sum_{i=1}^{N} (XT_i - \langle XT \rangle)(XE_i - \langle XE \rangle)}{(N - 1)(SXT)(SX})$$

(1)

Where $R$ is correlation coefficient and unit less, $\langle XT \rangle$ and $\langle XE \rangle$ are the mean theoretical and experimental reaction cross-sections respectively, $XT_i$ and $XE_i$ are the theoretical and experimental total cross-sections of the $i$th value respectively, $N$ is the number of the theoretical and experimental data, $SXT$ and $SX$ are the standard deviation of the theoretical and experimental total cross-sections respectively. If $0 < R < 0.3$, the correlation is weak and positive, $0.3 < R < 0.7$ describes moderate correlation and $0.7 < R < 1$, the correlation is strong.
and positive. This formulation is simple and convenient to find correlations between theory and experimental aspects of figures 1 to 3.

3. Results and discussions

3.1. The reaction channels of alpha and $^{209}$Bi

The calculated results of $^{209}$Bi ($\alpha$, $x$n) reaction cross-section using computer code COMPLET and the experimental data from EXFOR database are presented in tables 1 to 3 and figures 1 to 3 [10, 26]. Figures 1 to 3 show the agreement between the calculated results and the experimental one. All figures show plots of Energy (MeV) versus reaction cross-section (mb) for ($\alpha$, $x$n) reaction channels [15].

The maximum $^{209}$Bi ($\alpha$, $x$n) reaction cross-sections for each channel are very well predicted [19]. Level density parameter, probably related and very sensitive parameter, is an important factor in the calculation of cross-sections [10].

3.2. $^{209}$Bi ($\alpha$, n)$^{212}$At nuclear reaction

When $^{209}$Bi is bombarded by alpha particle, it can produce a neutron and a daughter particle $^{212}$At [10, 21]. Excitation functions for $^{209}$Bi ($\alpha$, n)$^{212}$At nuclear reaction are summarized in table 1 and plotted in figure 1. Figure 1 is the graph of projectile energy versus reaction cross-section for this reaction channel. The plots of reaction cross-section against the energy of the incident particle describes the Excitation function of the daughter product.

Where: $A$ is the graph of experimental reaction cross-section of $^{209}$Bi ($\alpha$, n)$^{212}$At, $B$ is the graph of compound reaction cross-section of $^{209}$Bi ($\alpha$, n)$^{212}$At, $C$ is the graph of pre compound reaction cross-section of $^{209}$Bi ($\alpha$, n)$^{212}$At.

From figure 1, both the theoretical pre equilibrium and equilibrium reaction cross-section evaluations of $^{209}$Bi ($\alpha$, n)$^{212}$At are in a good agreement with the experimental data in the energy range from 16 MeV to 20 MeV [18, 21]. At higher energies from 22.50 MeV to 23.50 MeV, the theoretical results have weak correlations to the experimental one. The computer code COMPLETE on areas of higher energies gives non-uniform nuclear data in consistent approach as shown in figure 1 [5]. The correlation coefficient of figure 1 for low energy ranges between the compound reaction cross-section mechanisms and the experimental data is $R = 0.898$, and between the pre–compound reaction cross section and the experimental data is: $R = 0.901$. Based on the correlation coefficient results, both the theoretical results show strong and positive correlation coefficients with the experimental one in this energy range.

3.3. $^{209}$Bi ($\alpha$, 2n)$^{211}$At nuclear reaction

When $^{209}$Bi is bombarded by alpha particle, it can produce $^{211}$At with two neutrons [8, 25]. Based on the EXFOR database and computer code COMPLETE, the results for ($\alpha$, 2n) reaction channel are tabulated as in table 2 [18, 19]. Figure 2 and table 2 show the excitation functions for the $^{209}$Bi ($\alpha$, 2n)$^{211}$At nuclear reaction. Figure 2 expressed the experimental and the theoretical excitation functions in the energy range of 21.10 MeV to 29.20 MeV of the channel.

For the given energy range, the experimental and the theoretical excitation functions of $^{209}$Bi ($\alpha$, 2n)$^{211}$At are plotted in figure 2.

Where: $A$ is the graph of experimental reaction cross-section of $^{209}$Bi ($\alpha$, 2n)$^{211}$At, $B$ is the graph of compound reaction cross-section of $^{209}$Bi ($\alpha$, 2n)$^{211}$At, $C$ is the graph of pre compound reaction cross-section of $^{209}$Bi ($\alpha$, 2n)$^{211}$At.

In figure 2, the compound nucleus reaction mechanism of $^{209}$Bi ($\alpha$, 2n)$^{211}$At in the energy range of 21.1 MeV to 23.1 MeV remains higher than the experimental one. The pre–compound nucleus reaction mechanism of $^{209}$Bi ($\alpha$, 2n)$^{211}$At in the energy range of 23.8 MeV to 29.2 MeV dominates. From figure 2, evaluations of reaction cross-section results of $^{209}$Bi ($\alpha$, 2n)$^{211}$At show an agreement between the experimental data [17, 24].

The correlation coefficient between the compound nucleus reaction cross-section mechanism and the experimental one has a coefficient of $R = 0.991$, and between the pre compound nucleus reaction cross section and the experimental one is $R = 0.991$. Hence, both the theoretical results show strong and positive correlation coefficient with the experimental one.

3.4. $^{209}$Bi ($\alpha$, 3n)$^{210}$At nuclear reaction

When $^{209}$Bi is bombarded by alpha particle, it can produce $^{210}$At with three neutrons [27, 28]. The results for $^{209}$Bi ($\alpha$, 3n)$^{210}$At from EXFOR data center and COMPLETE computer code are tabulated as in table 3 [18, 19]. The theoretical prediction and the measured data for $^{209}$Bi ($\alpha$, 3n)$^{210}$At nuclear reaction are shown in table 3 and plotted in figure 3.
Table 2. Results of the computer code COMPLET evaluation of $^{209}$Bi ($\alpha$, 2$n$)$^{211}$At cross section Compared with experimental data.

| Energy (MEV) | Reaction cross section (mb) | Pre-comp (mb) | Compound (mb) |
|--------------|----------------------------|---------------|---------------|
| 21.1         | 10.1                       | 77.1 ± 0.114  | 55.5 ± 0.134  |
| 21.4         | 12.8                       | 102.4 ± 0.099 | 81.8 ± 0.110  |
| 22.0         | 68.3                       | 195.6 ± 0.072 | 167.4 ± 0.077 |
| 22.2         | 72.2                       | 222.0 ± 0.067 | 197.1 ± 0.071 |
| 22.9         | 164.3                      | 323.3 ± 0.056 | 299.2 ± 0.058 |
| 23.1         | 195.0                      | 353.0 ± 0.053 | 333.5 ± 0.055 |
| 23.8         | 309.8                      | 463.7 ± 0.046 | 461.5 ± 0.046 |
| 24.0         | 348.8                      | 491.3 ± 0.045 | 493.4 ± 0.045 |
| 24.7         | 432.2                      | 578.8 ± 0.042 | 597.1 ± 0.041 |
| 24.8         | 450.5                      | 599.8 ± 0.041 | 614.0 ± 0.040 |
| 25.6         | 561.8                      | 692.7 ± 0.038 | 721.3 ± 0.037 |
| 26.4         | 589.6                      | 784.9 ± 0.036 | 819.9 ± 0.035 |
| 26.8         | 715.2                      | 823.6 ± 0.035 | 865.3 ± 0.034 |
| 27.7         | 761.1                      | 898.7 ± 0.033 | 946.3 ± 0.033 |
| 28.1         | 826.7                      | 935.1 ± 0.033 | 978.6 ± 0.032 |
| 28.4         | 837.7                      | 959.5 ± 0.032 | 1003 ± 0.032  |
| 29.2         | 906.5                      | 920.4 ± 0.033 | 949.1 ± 0.032 |

Table 3. Results of the Computer code COMPLET evaluation of $^{209}$Bi ($\alpha$, 3$n$)$^{210}$At cross section compared with experimental data.

| Energy (MEV) | Reaction cross section (mb) | Pre-comp (mb) |
|--------------|----------------------------|---------------|
| 29.0         | 36.10                      | 122.2 ± 0.090 | 71.4 ± 0.118  |
| 32.5         | 421.5                      | 791.4 ± 0.036 | 798.8 ± 0.035 |
| 35.7         | 796.6                      | 1088 ± 0.037  | 1370.0 ± 0.027|
| 38.7         | 939.7                      | 1170 ± 0.029  | 1559.0 ± 0.025|
| 41.6         | 785.6                      | 1035 ± 0.031  | 1349.0 ± 0.027|
| 44.2         | 570.2                      | 787.2 ± 0.035 | 783.4 ± 0.035 |
| 46.8         | 462.4                      | 566.7 ± 0.042 | 476.7 ± 0.046 |
| 49.2         | 392.6                      | 469.7 ± 0.046 | 209.6 ± 0.069 |
Table 3 shows that the energy of alpha particlees varies from 29.0 MeV to 49.2 MeV. Where; A is the graph of experimental reaction cross section of $^{209}$Bi ($\alpha$, 3n)$^{210}$At, B is the graph of compound reaction cross section of $^{209}$Bi ($\alpha$, 3n)$^{210}$At, C is the graph of pre compound reaction cross section of $^{209}$Bi ($\alpha$, 3n)$^{210}$At. All the reaction mechanisms (A, B and C) show quadratic behavior with a maxima alpha energy of 39 MeV. For alpha particle energies higher than 45.2 MeV, the pre-compound nucleus reaction mechanism is dominating [17, 18].

In figure 3, the cross–section results of $^{209}$Bi ($\alpha$, 3n)$^{210}$At show good agreements with the experimental data [17, 18]. The experimental data agree very well with the calculated results. The correlation coefficient between the compound nucleus reaction cross-section mechanism and the experimental one has a coefficient of $R = 0.973$, and between the pre compound nucleus reaction cross section and the experimental one is $R = 0.942$. Hence, both pre-equilibrium and equilibrium show strong and positive correlation with the experimental data.

3.5. General discussions
A validation of experimental data from EXFOR data library and the calculated result for ($\alpha$, n) ($\alpha$, 2n) and ($\alpha$, 3n) reaction channels using computer code COMPLET shows good agreement. These results in tables 1 to 3 and figures 1 to 3 from this research work demonstrated that the quality of the EXFOR database and computer code COMPLET are correlated [29].

The best level density parameter/calculation has been chosen for each reactions, and reaction cross-sections have been calculated with this level density parameter. All level density parameters/calculations have similar shapes and height with the experimental data taken from EXFOR database [13].

The shell structure effects are usually introduced as level density parameter dependence on the excitation functions. By varying the recommended level density parameters (8,9,10) and exciton numbers (4,5,6) the most theoretical values closest to the corresponding experimental one are taken to the analysis [2].

4. Conclusions
The theoretical expression of nuclear reaction cross-section in this research work confirmed that incident alpha-particle (charged and massive) must have sufficient energy to break the barrier in order to induce the equilibrium and pre-equilibrium effects on $^{209}$Bi ($\alpha$, n)$^{212}$At, $^{209}$Bi ($\alpha$, 2n)$^{211}$At, $^{209}$Bi ($\alpha$, 3n)$^{210}$At and $^{208}$Bi($\alpha$, xn)$^{212-8}$At reactions. These results could be useful in evaluating experimental values for $^{209}$Bi($\alpha$, xn) nuclear reaction and provide correct prediction of testing nuclear reaction cross-sections.

The simulated results using computer code COMPLET have been compared and confirmed to be in good agreement with the experimental values obtained using the EXFORE database. COMPLET code is a good tool for the prediction of nuclear reaction cross section, and this research work can be useful in the production of the radioisotopes of Bisthmus-209 and possible future needs.

Nuclear Reaction Data Center has played a crucial role for collection, exchange and dissemination of nuclear reaction data. The scope of EXFOR compilation has been extended from neutron-induced reaction cross sections to various projectiles and quantities, and today a large number of articles are newly scanned and added.
in a timely manner. We are trying to increase the quality of the database by removal of collection error and to improve accessibility for users.

In order to obtain a better agreement between the measured and calculated excitation functions, the level density parameters and exciton numbers were highly modified within the recommended limits. The comparisons for the reaction cross-section calculations have been performed by employing the experimental data between 10 MeV to 70 MeV.

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