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Evaluation of Excitation Functions of Reactions Used in Production of Some Medical Radioisotopes

Idris Ahmad*, **Yahya Ibrahim Yola**, **Fatima Salman Koki**

Department of Physics, Bayero University Kano, Kano, Nigeria
Email: *manidris37@yahoo.com

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Abstract

In this work, reaction cross-sections were calculated and Excitation Functions were evaluated for productions of ^{208}Bi, ^{212,211,210}At, ^{211,210}Po isotopes using EXIFON code in the energy range from 0 MeV to 30 MeV. The code is based on an analytical model for statistical multistep direct and multistep compound reactions (SMD/SMC model). This work also investigates the shell structure effect on the reaction cross-section, the results obtained show that the cross-sections of (a, na) reaction for both with shell correction and without shell correction are zeros at energies range considered, this shows that the energy of the incident particle is below the threshold of this reaction due to the present of coulomb repulsive force between the projectile and target nucleus.

Keywords

Nuclear Reaction, Cross-Section, Excitation Function, Radioisotope, Nuclear Model

1. Introduction

Studies of excitation functions of particle-induced reactions are of considerable significance for testing nuclear models as well as for practical applications, especially in cyclotron production of radioisotopes [1]. Nuclear reaction in the intermediate-energy region is a matter of interest in some fields of technology and science such as reactor technology, radiation therapy in nuclear medicine, medical radionuclide production, diagnostic and therapeutic studies, Accelerator Driven Systems , fusion and fission reactor. The artificially produced radioactive isotopes are important for many different applications [2] [3] [4] [5]. Radioactive isotopes play an important role in the field of medical science in terms of beneficial applications in both diagnosis and therapy purposes [6]. In radioisotope production programmers, nuclear reactions data are mainly needed for optimization of production routes [7] [8] [9]. The cross section data for different nuclide was intensively investigated and up to now, the nuclear databases are accessible online [10]-[22].

A nuclear reaction is a process that occurs when a nuclear particle (nucleon or nucleus) gets into close contact with another [23]. In the general case, an arbitrary number of particles may emerge. The probability of the reaction processes as a function of the energy of the incident particle, in the energy and the direction of the outgoing particles is usually interested in the whole set of reactions.

$$a + X = \begin{cases} X + a \\ X^* + a \\ Y + b \\ Z + c \\ etc \end{cases} \tag{1.1}$$

The first two reactions (1.1) are distinguished by the fact that the projectile re-emerges after the reaction. The first of these represents elastic scattering. The second reaction represents inelastic scattering.

To calculate the reaction cross section, it is necessary to compute the number of particles that disappear from the elastic channel, what is measured by the flux of the current of probability vector through a spherical surface of large radius centered at the target [24]

$$\sigma_r = \pi \bar{\lambda}^2 \sum_{l=0}^{\infty} (2l+1)\left(1 - |\eta_l|^2\right) \tag{1.2}$$

A radial wave function inside the nucleus should connect to the external function with a continuous function and its derivative at $r = R$.

$$f_l \equiv R\left[\frac{\mathrm{d}u/\mathrm{d}r}{u}\right]_{r=R} \tag{1.3}$$

The function must have identical values if calculated with the internal or the external function and this condition creates a relationship between f_l and η_l. Hence, the knowledge of f_l leads to the knowledge of the cross sections [24].

$$\sigma_{r,0} = \pi \bar{\lambda}^2 \frac{-4kRf_l}{f_R^2 + (f_l - kR)^2} \tag{1.4}$$

We have an equation that is useful when we study the presence of resonances in the excitation function (cross section as a function of the energy).

Statistical multistep model

Statistical multistep models are very successful in describing nuclear reactions at energies up to about 100 MeV [25]. These models enable the description of direct, pre-equilibrium, and equilibrium processes in a consistent way for a wide mass number range and various reaction channels, e.g. neutrons, protons, alpha-particles, and gamma-particles.

In the statistical multistep model, the total emission spectrum of the process

(a,xb) is divided into three main parts [14] [26],

$$\frac{d\sigma_{a,xb}(E_a)}{dE_b} = \frac{d\sigma_{a,b}^{\text{SMD}}(E_a)}{dE_b} + \frac{d\sigma_{a,b}^{\text{SMC}}(E_a)}{dE_b} + \frac{d\sigma_{a,xb}^{\text{MPE}}(E_a)}{dE_b} \tag{1.5}$$

The first term on the right hand side of Equation (1.5) represents the statistical multistep direct (SMD) part which contains from single-step up to five-step contributions. The second term represents the statistical multistep compound (SMC) emission which is based on a master equation. Both terms together (SMD + SMC) represents the first-chance emission process [27] [28]. The last term of Equation (1.5) represents the multiple particle emission (MPE) reaction which includes the second-chance, third-chance emissions, etc. These terms are summarized below:

$$\frac{d\sigma_{a,xb}^{\text{MPE}}(E_a)}{dE_b} = \sum_c \frac{d\sigma_{a,cb}(E_a)}{dE_b} + \sum_{c,d} \frac{d\sigma_{a,cdb}(E_a)}{dE_b} + \cdots \tag{1.6}$$

The following relations between the optical model (OM) reaction cross section and the energy-integrated partial cross sections should be satisfied (at each incident energy (E_a))

$$\sigma_a^{OM} = \sum_b \sigma_{a,b} \tag{1.7}$$

$$\sigma_{a,b} = \sum_c \sigma_{a,bc} \text{ and } \sigma_{a,bc} = \sum_d \sigma_{a,bcd} \tag{1.8}$$

With

$\sigma_{a,b} = \sigma_{a,b}^{\text{SMD}} + \sigma_{a,b}^{\text{SMC}}$ the total first-chance emission. In this context, activation cross sections are given by

$$\sigma_{a,b\gamma} = \sigma_{a,b} - \sum_{c\neq\gamma} \sigma_{a,bc} \tag{1.9}$$

$$\sigma_{a,cb\gamma} = \sigma_{a,cb} - \sum_{d\neq\gamma} \sigma_{a,cbd} \tag{1.10}$$

where $b,c,d \neq \gamma$

For example, the (n,p)-activation cross sections have the form

$$\sigma_{a,p\gamma} = \sigma_{n,p} - \sigma_{n,pn} - \sigma_{n,2p} - \sigma_{n,p\alpha} \tag{1.11}$$

The SMD cross section is a sum over s-step direct processes given by: [29]

$$\frac{d\sigma_{a,b}^{\text{SMD}}(E_a)}{dE_b} = \sum_{s=1} \frac{d\sigma_{a,b}^{s}(E_a)}{dE_b} \tag{1.12}$$

The SMD cross section has the form

$$\frac{d\sigma_{a,b}^{SMC}(E_a)}{dE_b} = \sigma_a^{SMC}(E_a) \sum_{N=N_0}^{N^I} \frac{\tau_N(E)}{\hbar} \sum_{(\Delta V)} \Gamma_{N,b}^{(\Delta V)}(E,E_b)\uparrow \tag{1.13}$$

where τ_N satisfies the time-integrated master equation

$$-\hbar\delta_{NN_0} = \Gamma_{N-2}^{(+)}(E)\downarrow \tau_{N-2}(E) + \Gamma_{N+2}^{(-)}(E)\downarrow \tau_{N+2}(E) - \Gamma_N(E)\tau_N(E) \tag{1.14}$$

and

$$\Gamma_N^{(\Delta v)}(E)\downarrow = 2\pi I_{SS}^2 \rho_N^{(\Delta v)}(E) \tag{1.15}$$

The multiple particle emission is expressed as:

$$\frac{\mathrm{d}\sigma_{a,xb}^{\mathrm{MPE}}\left(E_a\right)}{\mathrm{d}E_b}=\sum_c\frac{\mathrm{d}\sigma_{a,cb}\left(E_a\right)}{\mathrm{d}E_b}+\sum_{cd}\frac{\mathrm{d}\sigma_{a,cdb}\left(E_a\right)}{\mathrm{d}E_b}+\cdots \tag{1.16}$$

To keep the model tractable, a simple two-body interaction is assumed: [27]

$$I\left(r_1,r_2\right)=-4\pi\frac{F_0}{A}\left[\chi_{nl}\left(R\right)\right]^{-4}\delta\left(r_1-r_2\right)\delta\left(r_1-R\right) \tag{1.17}$$

$F_0=27.5\ \mathrm{MeV}$ taken from nuclear structure considerations.

The factor $\left[\chi_{nl}\left(R\right)\right]^{-4}$ contains the wave function at the nuclear radius $R=r_0A^{1/3}$

The single-particle state density of particles $C=n,p,\alpha$ with mass μ_c is given by

$$\rho\left(E_c\right)=\frac{4\pi V\mu_c\left(2\mu_cE_c\right)^{1/2}}{\left(2\pi\hbar\right)}=\left(4.48\times10^{-3}\ \mathrm{fm}^{-3}\cdot\mathrm{MeV}^{-3/2}\right)r_0^3AE_C^{1/2} \tag{1.18}$$

Where $V=\frac{4\pi R^3}{3}$ is equal to the nuclear volume [26].

The single-particle state density of bound particles (at Fermi energy) is then defined by

$$g=4\rho\left(E_F\right) \tag{1.19}$$

Where the factor 4 considers the spin and isospin degeneracy

2. Procedure

EXIFON code was used which is computer program package for computational nuclear Data physics which is based on an analytical model for statistical multistep direct and multistep compound reactions (SMD/SMC model). It predicts emission spectra, angular distributions, and activation cross sections for neutrons, protons, alpha particles, and photons. Multiple particle emissions are considered for up to three decays of the compound system. EXIFON is a fast, easy-to-handle code which predicts cross sections from one global parameter set. The only adjustable quantity is the pairing shift. The INPEXI code creates input files for EXIFON2.0 from mass and shell-correction tables. The MAKE6 code transforms EXIFON output into an ENDF-6 format file [26]. It is tested and recommended code by international atomic energy agency (IAEA).

The model is based on random matrix physics with the use of the Green's function formalism [29] [30]. All calculations are performed without any free parameters. Results were presented for bombarding energies below 30 MeV [31] [32].

2.1. Cross section Calculations

The program was run and the input and output directory was defined, and then the target nucleus is specified. The neutron was chooses as incident particle followed by selecting the target nucleus and excitation function in the general option section for this calculation.

The number of incident energy was specified followed by the first incident energy, and then the incident energy step is also specified. The cross section correspond to each particular energy was obtained.

2.2. Shell Structure Effects

The shell structure effects are considered in SMC processes. Under such a situation, the single-particle state density g, in Equation (1.19) is multiplied by the factors

$$\left(1+\frac{\delta W}{E_X}\left[1-\exp\left(-\gamma E_X\right)\right]\right) \tag{2.1}$$

With $\gamma = 0.05\,\text{MeV}^{-1}$ and δW as the shell correction energy taken from tables [33] where the quantity $E_X = E \text{ or } U$ which denotes the excitation energy of the composite or residual systems respectively.

The calculations in this study were performed with $(\delta W \neq 0)$ and without $(\delta W = 0)$ shell corrections. The procedures in 2.1 and 2.2 were repeated several times and the results of cross sections were obtained.

3. Results and Discursions

The cross section obtained was tabulated in hot-pot **Figures 1-3** and the excita-

with shell correction						without shell correction				
Energy	(a,a)	(a,na)	(a,ag)	(a,an)		Energy	(a,a)	(a,na)	(a,ag)	(a,an
1	0	0	0	0		1	0	0	0	0
2	0	0	0	0		2	0	0	0	0
3	0	0	0	0		3	0	0	0	0
4	0	0	0	0		4	0	0	0	0
5	0	0	0	0		5	0	0	0	0
6	0	0	0	0		6	0	0	0	0
7	0	0	0	0		7	0	0	0	0
8	0	0	0	0		8	0	0	0	0
9	0	0	0	0		9	0	0	0	0
10	0	0	0	0		10	0	0	0	0
11	0	0	0	0		11	0	0	0	0
12	0	0	0	0		12	0	0	0	0
13	0	0	0	0		13	0	0	0	0
14	0	0	0	0		14	0	0	0	0
15	0	0	0	0		15	0	0	0	0
16	0	0	0	0		16	0	0	0	0
17	0	0	0	0		17	0	0	0	0
18	0	0	0	0		18	0	0	0	0
19	0	0	0	0		19	0	0	0	0
20	0	0	0	0		20	0	0	0	0
21	0	0	0	0		21	0	0	0	0
22	0	0	0	0		22	0	0	0	0
23	0.1	0	0	0		23	0.1	0	0	0
24	0.2	0	0	0		24	0.2	0	0	0
25	0.4	0	0	0		25	0.4	0	0	0
26	0.6	0	0	0		26	0.6	0	0	0
27	0.9	0	0	0		27	0.9	0	0	0
28	1.1	0	1.1	0		28	1.2	0	1.2	0
29	1.4	0	1.4	0		29	1.4	0	1.4	0
30	1.7	0	1.6	0		30	1.7	0	1.6	0

Figure 1. Cross sections at different incident energies for (a, a), (a, na), (a, ag), (a, an) reactions.

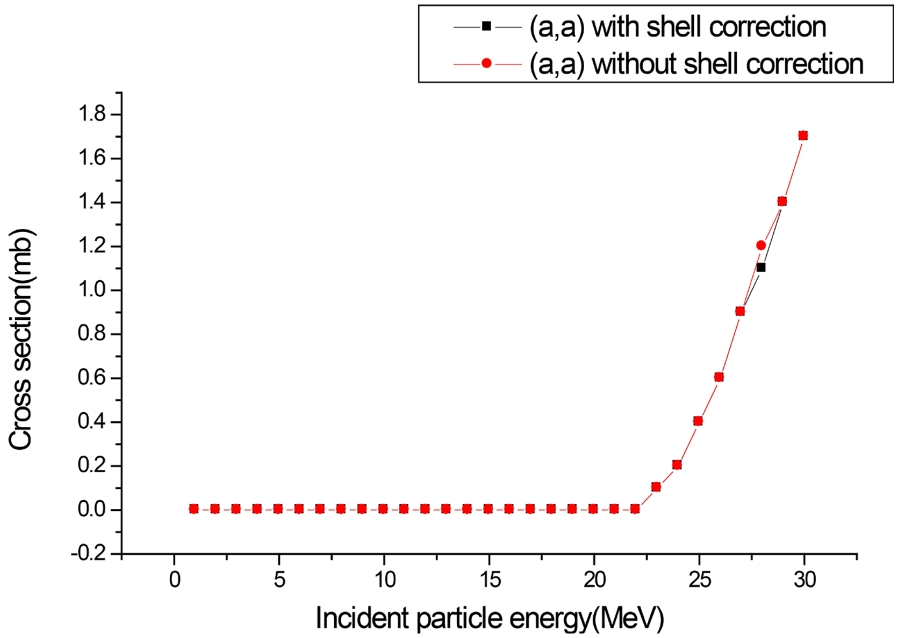

Figure 2. Excitation function ^{208}Bi(a,a) ^{208}Bi reaction.

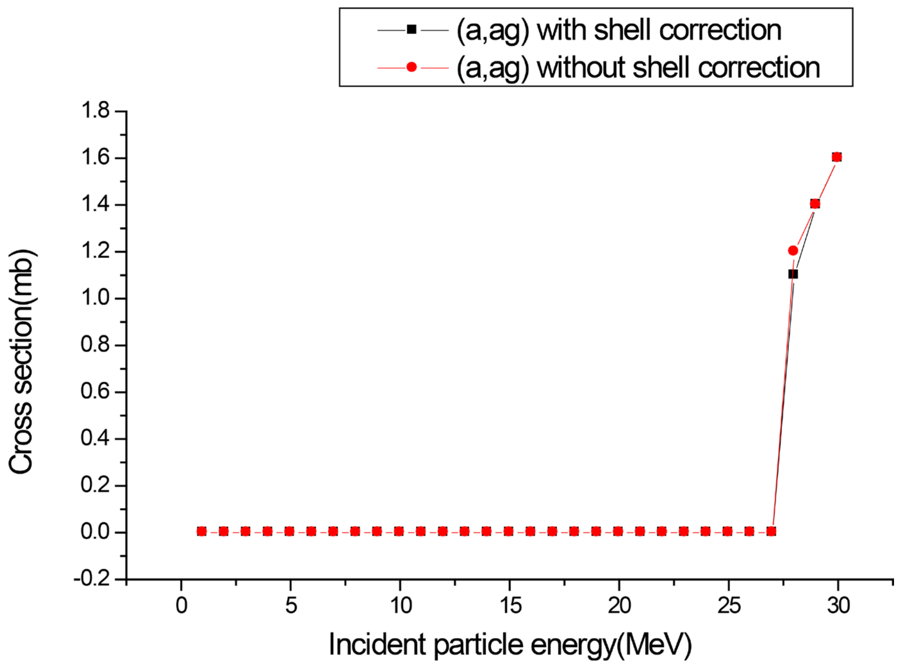

Figure 3. Excitation function ^{208}Bi(a,ag) ^{208}Bi reaction.

tion function was showed in Figures 1-10. The calculations in which the shell correction was taken into consideration are denoted by "With shell correction" on the graph's legend, while those without the shell correction effects are denoted by "Without shell correction".

In hot-pot Figure 1, One can observe that the cross sections for ^{208}Bi(a, na)^{207}Bi and ^{208}Bi(a, an)^{207}Bi reactions are zeros. This shows that these two reactions would not occur at the incident energy of (0 - 30) MeV.

Figure 2 and Figure 3 are graphs of cross section against incident energy of the alpha particle,

The two reactions are distinguished by the fact that the projectile re-emerges after the reaction. The first of these represents elastic scattering. The second reaction represents inelastic scattering in Equation (2.3).

with shell correction						without shell correction				
Energy	(a,g)	(a,ng)	(a,pg)	(a,2ng)		Energy	(a,g)	(a,ng)	(a,pg)	(a,2ng)
1	0	0	0	0		1	0	0	0	0
2	0	0	0	0		2	0	0	0	0
3	0	0	0	0		3	0	0	0	0
4	0	0	0	0		4	0	0	0	0
5	0	0	0	0		5	0	0	0	0
6	0	0	0	0		6	0	0	0	0
7	0	0	0	0		7	0	0	0	0
8	0	0	0	0		8	0	0	0	0
9	0	0	0	0		9	0	0	0	0
10	0	0	0	0		10	0	0	0	0
11	0	0	0	0		11	0	0	0	0
12	0	0	0	0		12	0	0	0	0
13	0	0	0	0		13	0	0	0	0
14	0	0	0	0		14	0	0	0	0
15	0	0	0	0		15	0	0	0	0
16	0	0	0	0		16	0	0	0	0
17	0	0	0	0		17	0	0	0	0
18	0	0	0	0		18	0	0	0	0
19	0	3.2	0	0		19	0	3.2	0	0
20	0	59.8	0	0		20	0	59.8	0	0
21	0	135.2	0	0		21	0	135.2	0	0
22	0.1	229.3	0	0		22	0.1	229.3	0	0
23	0.3	341.9	0	0.1		23	0.3	342	0	0
24	0.4	471	0.1	1.2		24	0.4	471.8	0.1	0.3
25	0.6	592.7	0.2	5.8		25	0.6	596.7	0.2	1.8
26	0.7	695.5	0.4	19.5		26	0.7	708	0.4	7.1
27	0.9	771.9	0.6	50.9		27	0.8	801.5	0.6	21.2
28	1	815.1	0.9	107.5		28	0.9	870.8	1	51.8
29	1	820.8	1.4	194.5		29	1	906.9	1.4	108.4
30	1.1	793.2	1.8	306.7		30	1.1	908.7	1.9	192.6

Figure 4. Cross sections at different incident energies for (a, g), (a, ng), (a, pg), (a, 2ng) reactions.

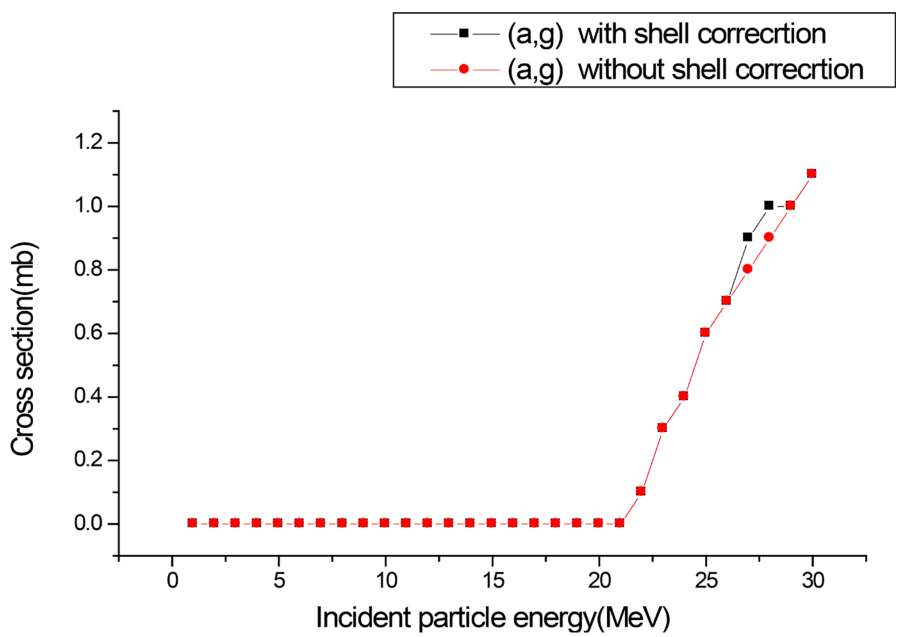

Figure 5. Excitation function $^{208}Bi(a, g)^{212}At$ reaction.

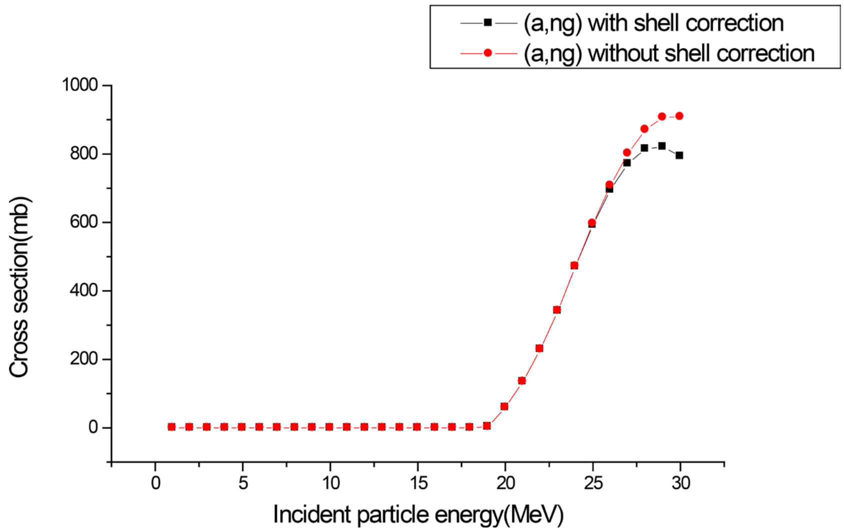

Figure 6. Excitation function $^{208}Bi(a, ng)^{211}At$ reaction.

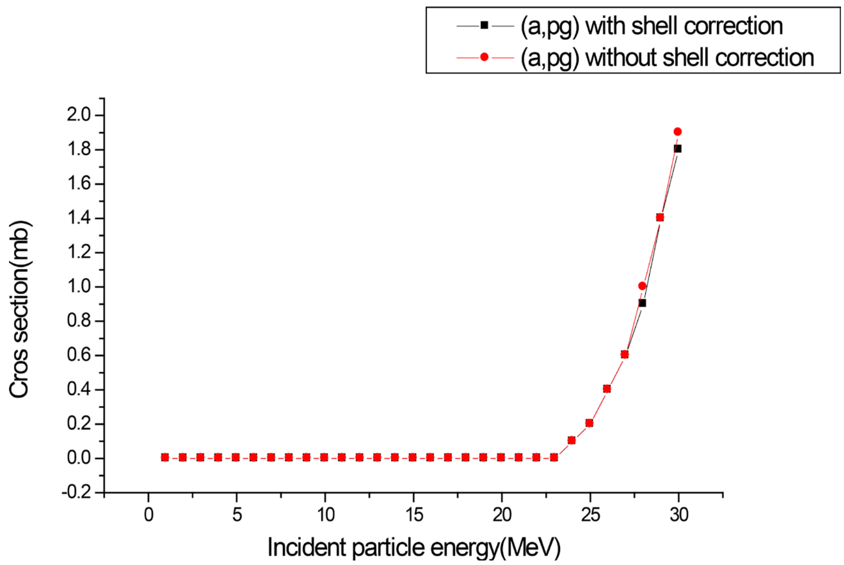

Figure 7. Excitation function $^{208}Bi(a, pg)^{211}Po$ reaction.

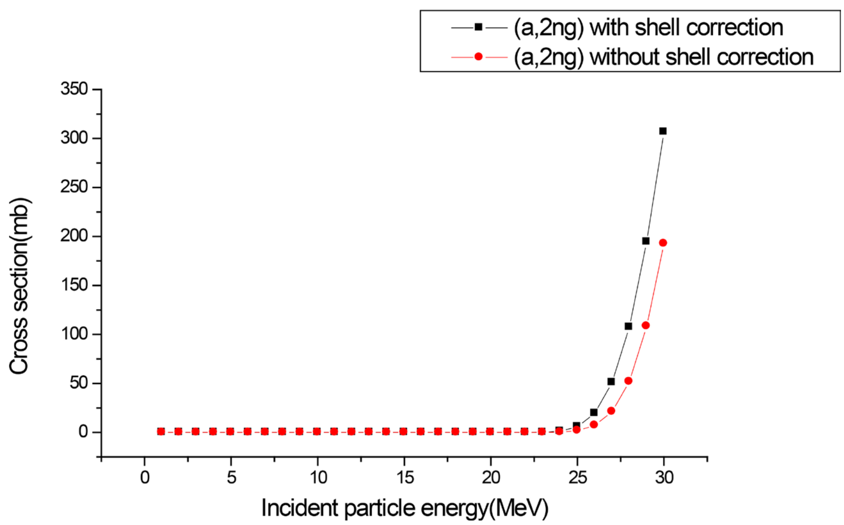

Figure 8. Excitation function $^{208}Bi(a, 2ng)^{210}At$ reaction.

with shell correction						without shell correction				
Energy	(a,n)	(a,2n)	(a,pn)	(a,3n		Energy	(a,n)	(a,2n)	(a,pn)	(a,3n)
1	0	0	0	0		1	0	0	0	0
2	0	0	0	0		2	0	0	0	0
3	0	0	0	0		3	0	0	0	0
4	0	0	0	0		4	0	0	0	0
5	0	0	0	0		5	0	0	0	0
6	0	0	0	0		6	0	0	0	0
7	0	0	0	0		7	0	0	0	0
8	0	0	0	0		8	0	0	0	0
9	0	0	0	0		9	0	0	0	0
10	0	0	0	0		10	0	0	0	0
11	0	0	0	0		11	0	0	0	0
12	0	0	0	0		12	0	0	0	0
13	0	0	0	0		13	0	0	0	0
14	0	0	0	0		14	0	0	0	0
15	0	0	0	0		15	0	0	0	0
16	0	0	0	0		16	0	0	0	0
17	0	0	0	0		17	0	0	0	0
18	0	0	0	0		18	0	0	0	0
19	3.2	0	0	0		19	3.2	0	0	0
20	59.8	0	0	0		20	59.8	0	0	0
21	135.2	0	0	0		21	135.2	0	0	0
22	229.3	0	0	0		22	229.3	0	0	0
23	342.1	0.1	0	0		23	342.1	0	0	0
24	472.1	1.2	0	0		24	472.1	0.3	0	0
25	598.6	5.8	0	0		25	598.6	1.8	0	0
26	715.1	19.5	0	0		26	715.1	7.1	0	0
27	822.7	50.9	0	0		27	822.7	21.2	0	0
28	922.6	107.5	0	0		28	922.5	51.8	0	0
29	1015.3	194.5	0.1	0		29	1015.3	108.4	0.1	0
30	1101.7	308.5	0.2	1.7		30	1101.6	192.9	0.2	0.4

Figure 9. Cross sections at different incident energies for (a, n), (a, 2n), (a ,pn), (a, 3n) reactions.

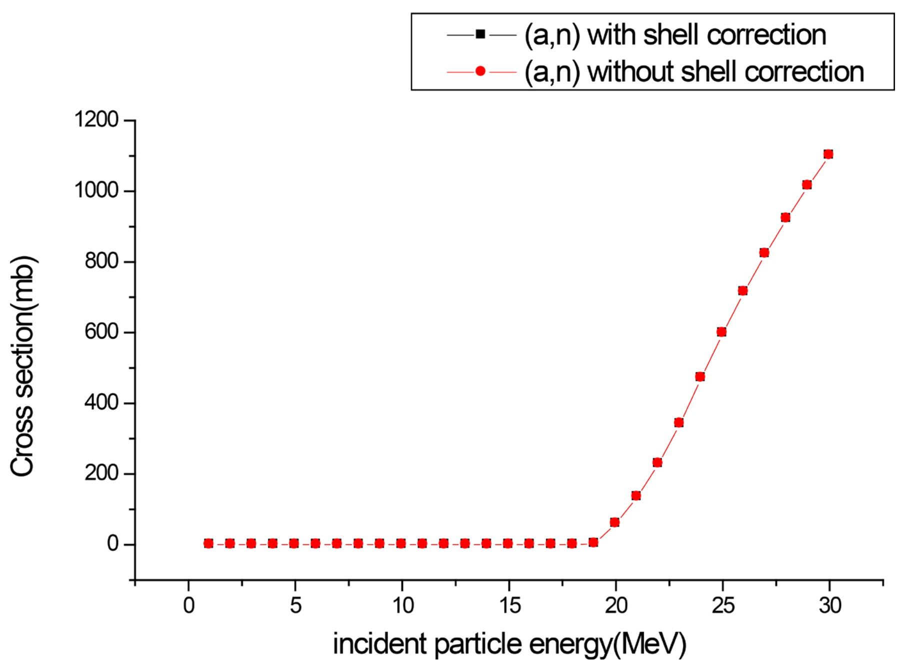

Figure 10. Excitation function ^{208}Bi(a, n)^{211}At reaction.

Figures 5-8 are graphs of cross section against incident energy of the alpha particle, $^{208}Bi(a, g)^{212}At$ is a compound nucleus formation of Astatine(212) followed by gamma emission. $^{208}Bi(a, ng)^{211}At$ is a knock out reaction for the nucleus formation of Astatine (211) followed by gamma emission. $^{208}Bi(a, pg)^{211}Po$ is also a knock out reaction for the nucleus formation of Polonium (211) followed by gamma emission. $^{208}Bi(a, 2ng)^{210}At$ is also a knock out reaction for the nucleus formation of Astatine(210) followed by gamma emission. All the results shows that shell structure correction does not much changes at the range of energies from (0 - 30) MeV.

Figures 10-13 are graphs of cross section against incident energy of the alpha particle, $^{208}Bi(a, n)^{211}At$ is a knock out reaction for the nucleus formation of Astatine (211). $^{208}Bi(a ,2n)$ ^{210}At is also a knock out reaction for the nucleus formation of Astatine (210) $^{208}Bi(a, pn)^{210}Po$ is also a knock out reaction for the nucleus formation of Polonium (210). $^{208}Bi(a, 3n)^{211}At$ is a knock out reaction for the nucleus formation of Astatine (209) All the results shows that shell structure correction does not much changes at the range of energies from (0 - 30) MeV except for $^{208}Bi(a, 3n)$ ^{212}At reaction although the cross section value is very small.

4. Conclusion

Nuclear reaction in the intermediate-energy region is a matter of interest in some fields of technology and science such as reactor technology, radiation therapy in nuclear medicine, medical radionuclide production, diagnostic and therapeutic studies, Accelerator Driven Systems (ADS), fusion and fission reactor. Radioactive isotopes play an important role in the field of medical

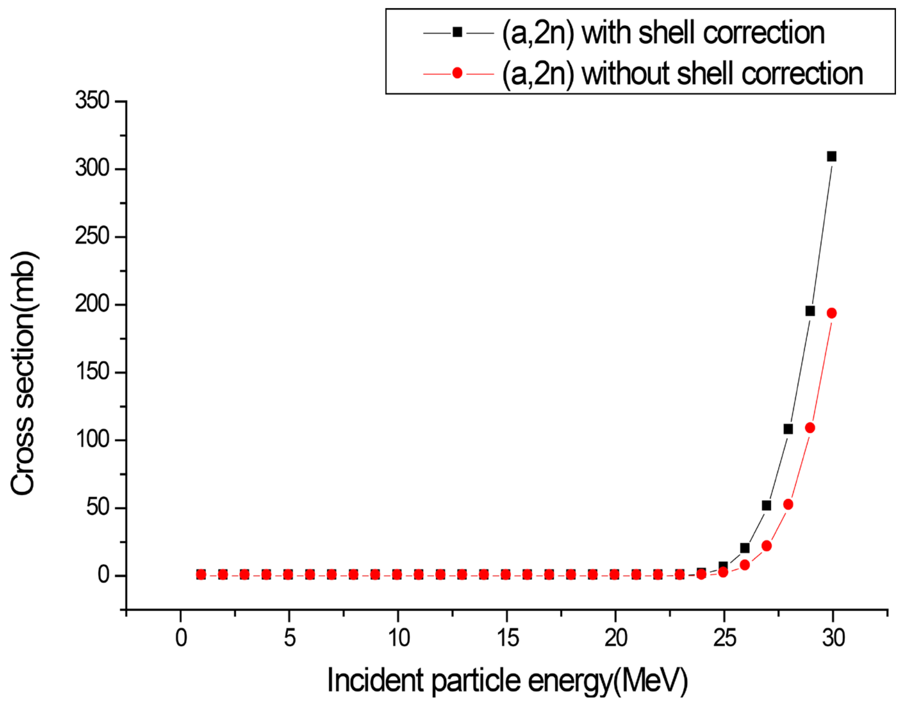

Figure 11. Excitation function $^{208}Bi(a, 2n)^{210}At$ reaction.

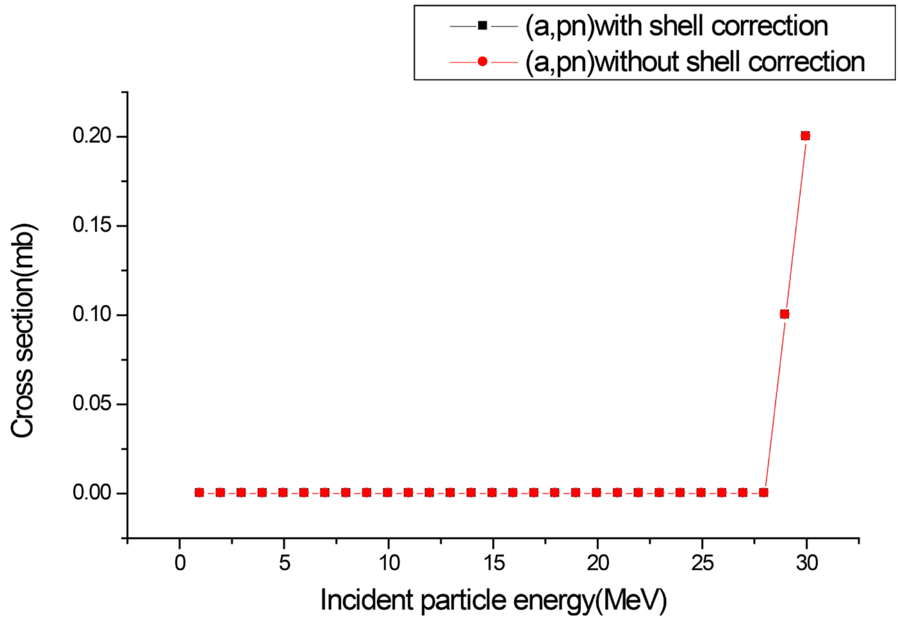

Figure 12. Excitation function ^{208}Bi(a, pn)^{210}Po reaction.

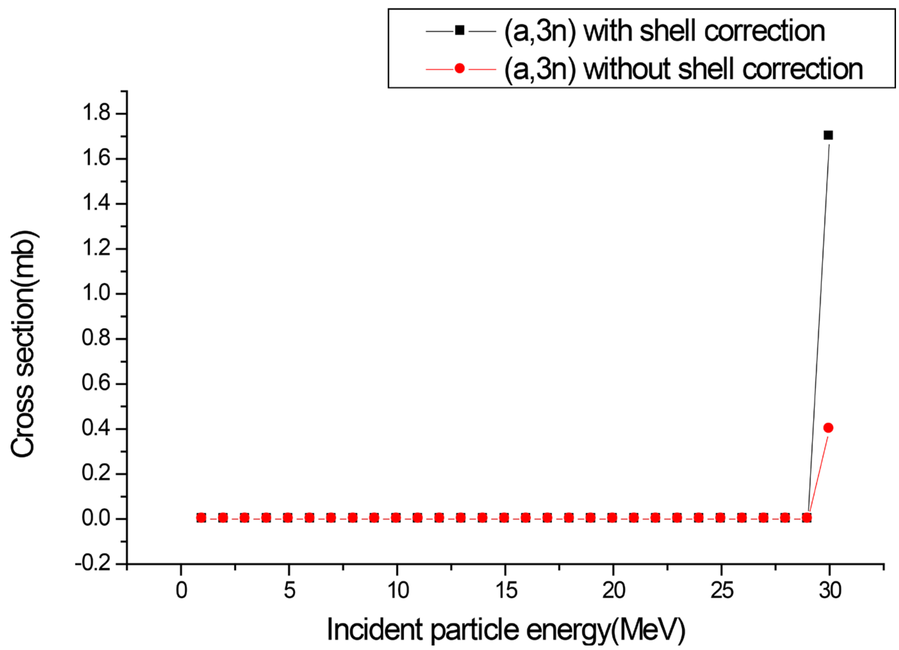

Figure 13. Excitation function ^{208}Bi(a, 3n) ^{212}At reaction.

science in terms of beneficial applications in both diagnosis and therapy purposes. The reaction cross-sections were calculated and Excitation Functions were evaluated for productions of ^{208}Bi, ^{212,211,210}At, ^{211,210}Po isotopes in the energy range from 0 MeV to 30 MeV. We also investigate the shell structure effect on the reaction cross-section, the results obtained show that the cross-section of (a, na) reaction for both with shell correction and without shell correction are zeros at energies range considered, this shows that the energy of the incident particle is below the threshold of this reaction due to the present of coulomb repulsive force between the projectile and target nucleus. The application in precise evaluation of the Excitation Functions as well as the production of isotopes is necessary to embrace the current and future needs for medical radionuclide.

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