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Analysis of Proton Induced Reactions on Yttrium Isotope Using Computer Code COMPLET

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Abstract: The variation of nuclear reaction cross-sections with the variation in projectile energies is called excitation functions has been a subject of great interest since last few decades. They beautifully display the pre-equilibrium as well as equilibrium emission of particles. The phenomenological pre-equilibrium models introduced to describe the equilibration process of an excited nucleus and the subsequent emission of particles have become a promising tool for the description, analysis and interpretation of nuclear reactions of energy greater than a few tens of MeV. In the study that is presented here proton induced reactions on the target element yttrium isotope were studied upto 80 MeV. The excitation functions for the five reactions of the type $89_Y(p, xn)$; x=2-4, $89_Y(p, xn)$; x=1, 2 were studied using the computer code COMPLET. The aim of this study is to analyze the nuclear reaction of yttrium isotope induced by proton particle using computer code COMPLET and EXFOR database. The corresponding experimental data were taken from EXFOR library. The calculated theoretical values were compared with the experimental results. It is observed that the calculated theoretical values show a systematic underestimated result for initial exciton configuration n_o=1(1p+0h) and level density parameter ACN/10 especially in multiparticle emissions. Hence, n_o=1(1p+0h) was less convenient choice for higher energies but low energy requirement makes this calculation better choice.

Keywords: Production Cross-Section, Code COMPLET, Nuclear Level Density, Exciton, Target Yttrium Isotope

1. Introduction

Analysis of the cross-section of proton-induced nuclear reaction is of interest in several fields. Proton-induced nuclear reactions in the incident energy range are commonly used for the production of radionuclides with minimal contamination, making them a production route for diagnostic and therapeutic medical radionuclides [1–3]. Nuclear reactions induced by medium energy projectiles (10-200MeV), were studied to understand the pre-equilibrium and compound nucleus reactions [4–7]. A priori knowledge of the excitation functions is essential to explain the compound nucleus and pre-equilibrium emission of particles in $(p, xnpn)$ reactions, to test the inadequacies of the various nuclear models developed during the last few decades [8–12], and to explain the underlying physics. Nuclear data play an essential role in the choice of a radioisotope for a medical application.

Nuclear structure and decay data determine the suitability of a radioisotope for diagnostic applications [1], while nuclear reaction data are used to study the possibility of its production in a pure form. The cross-section data on the proton-induced reaction of the target isotope yttrium (Y) are important for thin layer activation analysis (TLA), dose estimation, radiation protection in accelerator technology and a variety of this applications in nuclear medicine. Moreover, it is also useful to test the nuclear reaction mechanism because Yttrium is an atypical mono-isotopic element (Y has many isotopes from A=76-111) situated in the middle of rare –earth metals of the periodic table and ideally suitable for such studies [13–15]. The isotopes of yttrium and zirconium radionuclides $(88, 87, 86_{Zr}\ and\ 88, 87_{Y})$ produced from the

$Y(p,x) and\ Y(p,px)$reactions can also be used in the field of tumor diagnosis, therapy and in positron and photon emission tomography [16–18].

In this context, the present analysis of reaction cross sections was undertaken with two aims: The first one is to improve the quality of existing data, measured about a decade ago and also to enhance the reliability of pre-equilibrium exciton models. The second aim is to compare the experimental results obtained with one of the latest available theoretical codes [19] for the first time, in the energy that ranges between 10-80MeV. Thus, there is a strong motivation in the present work to calculate the excitation functions of five reactions in the above-mentioned energy range.

2. Materials and Methods

2.1. Calculations and Simulation Techniques Using Computer Code COMPLET

To check the behavior of the excitation function as well as the consistency and reliability of experimental data, various nuclear model calculations were performed using the code COMPLET [20]. To obtain a convention between the experimental & theoretical excitation functions as accelerate as possible, different input nuclear model parameters were adjusted. Besides, to check the reliability of the existing experimental data, the calculations were done to obtain the excitation functions over energy region where no experimental data were available.

The computer code COMPLET was used for the calculation of $88, 87, 86_{Zr}\ and\ 88, 87_{Y}$ in the $89_{Y}(p, x)$ (where x=2-4) and $(p, pn\ and\ p, p2n)$ were nuclear reactions cross-section induced from projectile energy range of 10-80 MeV. The calculated results were compared with the experimental values taken from the EXFOR database [21–23]. EXFOR and COMPLET were preferable in order to gather the experimental & the theoretical data respectively.

2.2. Computer Code COMPLET

The computer code COMPLET is a nuclear reaction code which was developed to generate theoretical data on nuclear reaction. Code COMPLET has been essentially developed to analyze the nuclear reaction mechanisms. The code COMPLET is an improved version of the earlier nuclear reaction codes of ALICE and is very important for several technical applications when the experimental data are not available or when it is impossible to measure the reaction cross-sections due to the experimental difficulties. The pre-equilibrium calculations in this code maybe performed in the framework of hybrid [24–26] model or geometry dependent hybrid [27] model. Very few parameters are required to get input data for pre-equilibrium and compound calculations. The input data are required to verify neutron and proton number of the target and projectile, i.e. the initial exciton number $n_o$and level density parameter a [26, 28]. In pre-equilibrium emission calculations the mentioned parameters are a pivotal quantity. COMPLET code helps to predict and investigate the value of the excitation functions of pure equilibrium decay as well as pre-equilibrium decay. The code COMPLET allows the evaporation of proton, neutron, deuterium and alpha particles, triton and Helium-3 [29, 30].

2.3. Experimental Results

The production cross-sections of the proton-induced reaction on 89_{Y} are available in the Experimental Nuclear Reaction Data Library (EXFOR) [21]. In the reaction $89_{Y}(p, 2n)88_{Zr}, 89_{Y}(p, 3n)87_{Zr}\ and\ 89_{Y}(p, 4n)86_{Zr},$ the product nuclei is the same, so all the decay parameters are the same and they differ in half-life, energies of emitted particles etc. The experimental data of the above-mentioned reactions were taken from [14, 15, 17, 31, 32]. EXFOR, IAEA nuclear science and technology.

2.4. Data Analysis Procedure

The data of this work were arranged in proper orders and organized by using tabulation (Tables 1-5) method. These organized data are described graphically with the help of origin software and spreadsheet and they are analyzed and interpreted accordingly by comparing with the measured experimental data.

3. Results and Discussion

The calculation data of the production of cross section of the $88{,}87{,}86_{Zr}\ and\ 88.87_{Y}$ in the $89_{Y}(p, x)$(where x=2-4), $(p, pn\ and\ p, p2n)$ reactions of nuclear processes are presented in Tables 1-5 and discussed in the subsequent subsections. The measured numerical cross-sections and their overall uncertainties are also presented in a table. The excitation functions of the produced radionuclides are presented in Figures 1-5 together (compared) with the experimental data available in EXFOR data center. In addition, since the input parameter is very important factor in Fermi gas formula, we varied this parameter to achieve the required result of the code COMPLET nuclear model for the purpose of isotope formation processes mentioned above. For this reason, the reaction cross-sections were calculated repeatedly by increasing and decreasing an input parameter factor. These variations were compared with each other to adjust the desired amount of input parameter for the experimental data.

The theoretical calculations were done by taking the initial exciton at $n_0 = 1$ with configurations $(1p + 0h)$ and the level density parameter $PLD, ACN/k = 10$ and they were checked to ensure and know their effects on the calculated values of excitation functions.

3.1. Determination of Production of Reaction Cross Section

3.1.1. The $\mathbf{89_{Y}(p, 2n)88_{Zr}}$ Process

All the calculated results agreed well with one another. The measured values were too much high at the beginning of energy and did not agreed with the calculated values. Around 41 MeV of energy and above, the theoretical results at $n_0 = 1$

values were going to zero and far apart to the experimental results. The experimental and theoretical values are thus comparable at the higher energy. This experimental value is much higher to the theoretical ($n_0 = 1$) reaction cross sections at the starting point of energy. The measured experimental values by [31] are higher than with our calculated values up to 51 MeV. For the calculated theoretical nucleus reaction at $n_0 = 1$, all those values were slightly lower than the experimental, but this is expected in higher energy there is no formation of less exciton numbers ($n_0 = 1$) nucleus reactions. The correlation of the theoretical & experimental excitation functions is strong and positive with the values of R=0.94 with the total exciton number $n_0 = 1$.

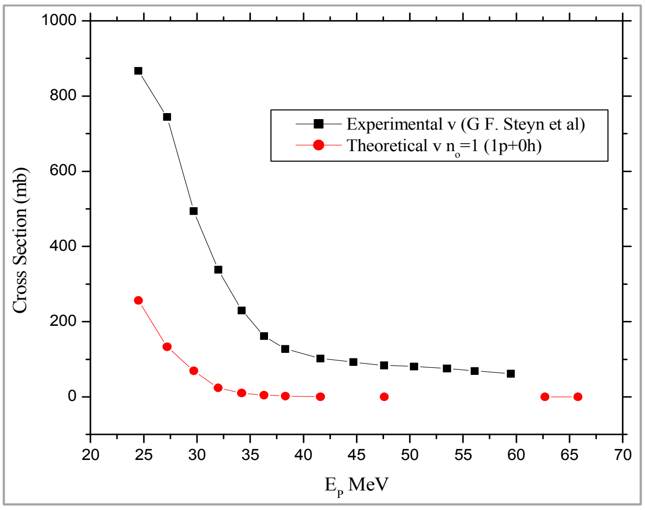

Figure 1. *Total cross-section against projectile energy of the reaction* $89_Y(p,2n)$ *for the experimental and calculated results.*

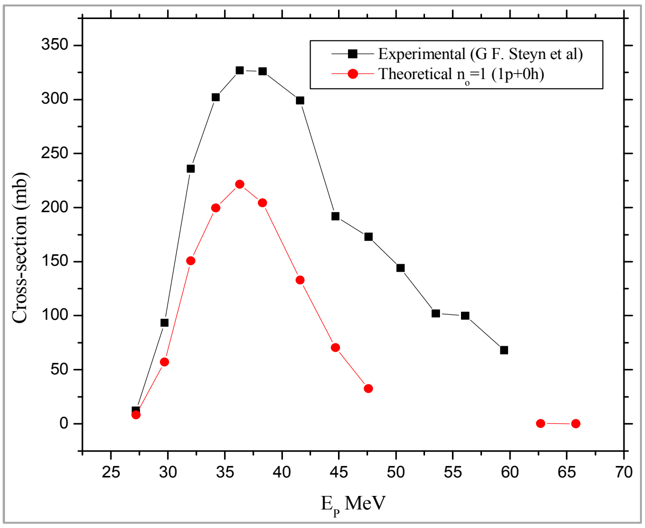

Figure 2. *Total cross-section against projectile energy of the reaction* $89_Y(p,3n)$ *for the experimental and calculated results.*

Table 1. *Theoretical and experimental total cross-section depends on projectile energy of* $89_Y(p,2n)$ *reactions.*

Proton Energy in (MeV)	Total cross-section (mb)	
	Experimental data	Theoretical value
65.8±0.3	58±4.12	0.0001321
62.7±0.3	59.1±4.19	0.0003821
59.5±0.4	61.6±4.3	0.001194
56.1±0.4	69.2±4.8	0.003504
53.5±0.5	75.5±5.3	0.01068
50.4 ±0.5	80.7±5.6	0.01772
47.6±0.5	83.8±5.9	0.05543
44.7±0.6	92.4±6.5	0.1806
41.6±0.6	102±7.1	0.6372
38.3±0.7	128±9	2.077
36.3±0.7	162±11.3	4.660
34.2±0.5	230±16.1	10.34
32±0.5	338±23.7	23.97
29.7±0.4	494±34.6	69.25
27.2±0.4	744±52.1	133.4
24.5±1	867±60.7	256.5

Table 2. *Theoretical and experimental total cross-section depends on projectile energy of* $89_Y(p,3n)$ *reactions.*

Proton Energy in (MeV)	Total cross-section (mb)	
	Experimental data	Theoretical value
65.8±0.3	68.5±6.6	0.1333
62.7±0.36	71.3±9.3	0.3400
59.5±0.41	68.2±8.6	0.8660
56.1±0.46	99.9±14.3	2.247
53.5±0.51	102±10.4	5.613
50.4±0.55	144±17.4	13.62
47.6±0.59	173±16.4	32.53
44.7±0.63	192±20.4	70.53
41.6±0.68	299±24.3	132.9
38.3±0.74	326±27.6	204.4
36.3±0.78	327±25.6	221.6
34.2±0.82	302±25.2	199.7
32±0.86	236±90.2	150.7
29.7±0.92	93.5±9.9	57.21
27.2±0.98	12.1±3.4	8.257

Table 3. *Theoretical and experimental total cross-section depends on projectile energy of* $89_Y(p,4n)$ *reactions.*

Proton Energy in (MeV)	Total cross-section (mb)	
	Experimental data	Theoretical value
66.6±0.2	38.2±2.5	1.189
65.4±0.2	41.4±2.7	1.498
64.2±0.2	45.5±2.9	1.835
61.6±0.2	55±3.6	3.545
59±0.2	63±4.1	4.895
56.4±0.2	73.6±4.8	6.590
53.6±0.3	79.6±5	8.641
52.1±0.3	76.8±5	8.551
50.2±0.3	65.4±4.4	7.382
48.4±0.3	57.5±3.9	4.567
46.5±0.3	43.1±2.9	2.246
44.7±0.3	23.9±1.6	1.060
42.7±0.3	9.2±0.6	0.2408
40.7±0.3	1.62±0.14	0.02072

Table 4. *Theoretical and experimental total cross-section depends on projectile energy of* $89_Y(p,p+2n)$ *reactions.*

Proton Energy in (MeV)	Total cross-section (mb)	
	Experimental data	Theoretical value
66.6±0.2	422.6±27.7	1.195
65.4±0.2	443.3±29	1.590
64.2±0.2	456.9±29.9	2.140
61.6±0.2	480.3±31.4	5.204
59±0.2	485.1±31.7	9.540

Proton Energy in (MeV)	Total cross-section (mb)	
	Experimental data	Theoretical value
56.4±0.2	528.7±34.2	22.86
53.6±0.3	573.8±37.5	52.53
52.1±0.3	602.7±39.4	69
50.2±0.3	708±48	118.5
48.4±0.3	835.9±56.4	196.8
46.5±0.3	952.1±66.3	305.1
44.7±0.3	1072.4±73.6	360.1
42.7±0.3	1131.9±76.35	525.6
40.7±0.3	1173.3±79.1	704
38.6±0.3	1158.38±78	829.7
36.4 ±0.3	1055±71.1	878.8

Table 5. *Theoretical and experimental total cross-section depends on projectile energy of* $89_Y(p, pn)$ *reactions.*

Proton Energy in (MeV)	Total cross-section (mb)	
	Experimental data	Theoretical value
79.6	133.6±25.8	0.00001309
75.4	139.9±15.4	0.00006209
70.9	142.3±15.6	0.0003689
66.2	144.6±15.9	0.001505
61.2	146.7±16.1	0.008518
57	152.8±16.5	0.03617
52.6	151.8±16.6	0.2197
49.4	193.7±21.7	0.6757
48	162.5±17.7	0.9817
45.4	201.3±21.9	2.987
42.7	170.1±18.5	8.960
40.6	209.4±22.8	19.27
36.9	215.4±23.4	81.96
34.4	272.4±29.5	160.4
26.4	280.2±30.4	858.9

3.1.2. The $89_Y(p, 3n)87_{Zr}$ *Process*

The calculated theoretical and the measured experimental excitation functions gave consistent results. In $89_Y(p, 3n)87_{Zr}$ reaction the reaction cross-sections results reached a maximum peak at 36 MeV in both the measured and the calculated excitation functions with different results. From figure 2, it is seen that the calculated data ($n_0 = 1$) are better at the beginning energy ranges and then after the increasing of energy the value decreased and the agreement was far from the experimental data. Around 44 MeV, the calculated data seem overlapping each other. The correlation between the experimental and the theoretical values at the total exciton $n_0 = 1$ nuclear reaction cross-section was positive and strong with a value of R=0.93.

3.1.3. The $89_Y(p, 4n)86_{Zr}$ *Process*

As shown in figure 3, the calculated results of the theoretical nucleus reactions are with total agreement and are far away from the measured experimental results at a given energies. Whereas the calculations from COMPLET code, the exciton number at $n_0 = 1$ nucleus formation, are negligible as compared to the experimental results at lower as well as higher energies. The experimental result is larger than the theoretical calculations at higher energies. This difference in the experimental and theoretical calculations clearly indicates that for the larger number of neutron emissions, a high amount of proton energy is needed. Both the theoretical value predications strongly underestimated the experiments above 40 MeV. Also, the theoretical model codes estimate the first maximum result almost correctly, but give different values after 42 MeV.

The results of the code COMPLET model to predict cross-sections were not in a good agreement with the experimental results reported by [15] EXFOR. The calculated values ($n_0 = 1$) relatively does not show a similar shape to the experimental results. The experimental data indicate higher magnitudes in the peak energy status. Both calculated & the measured values have strong and positive correlations with R=0.91 for $n_0 = 1$ and experimental values.

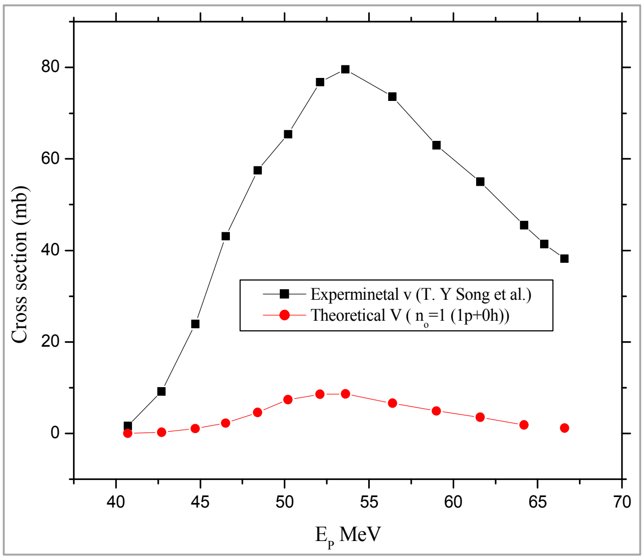

Figure 3. *Total cross-section against projectile energy of the reaction* $89_Y(p, 4n)$ *for the experimental and calculated results.*

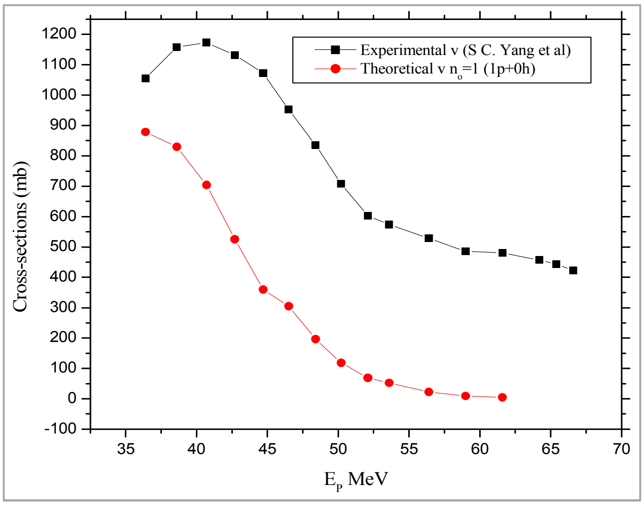

Figure 4. *Total cross-section against projectile energy of the reaction* $89_Y(p, p2n)$ *for the experimental and calculated results.*

3.1.4. The $89_Y(p, p + 2n)87_Y$ *Process*

89_{Zr} is produced exclusively from the 89_Y target isotope with a proton plus two neutron emissions. Table 4 indicates that the theoretical result ($n_0 = 1$) reached a maximum peak with 878.8mb at the energy range of 36 MeV and at different energy ranges (40 MeV) the experimental result also attained the peak 1173.3mb.

The calculated theoretical results are not comparable (i.e.

$n_0 = 1$) because they are in the energy range above 45 MeV though they give the same trend and values up to 66 MeV. The theoretical results at $n_0 = 1$ from code COMPLET did not seem to be a better approximation. The results are presented in figure 4.

The exciton number for $n_0 = 1$ with the experimental results show strong and positive correlation with R=0.90 values.

3.1.5. The $89_Y(p,pn)88_Y$ Process

At the beginning of projectile energy 26 MeV, the calculated theoretical values $n_0 = 1$ of the excitation functions were higher and the measured experimental results were lower than the calculated theoretical data. In fact, the theoretical and the experimental excitation functions attained a maximum peak at this same energy ranges.

The experimental cross-sections from EXFOR, IAEA database deduced for the $89_Y(p,pn)88_Y$ monitor reaction was compared with the theoretical calculated cross-section. After 48 MeV the exciton number which is $n_0 = 1$, nucleus reaction had zero value which was far from the measured experimental value and from the rest of theoretical reaction cross sections. For the increasing projectile energy both the experimental and theoretical reaction cross-section value decreased. Moreover, formations of excitation functions were not found at higher energy projectiles in $n_0 = 1$. The discrepancy in experimentally measured cross sections and theoretically calculated ones was insignificant.

The measured and calculated excitation functions showed a strong and positive correlation for the experimental value with $n_0 = 1$ were R=0.70 is moderate and also strong correlations.

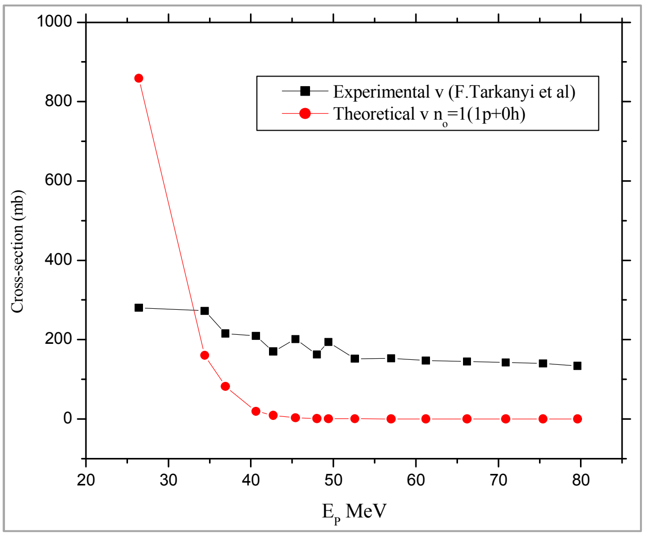

Figure 5. *Total cross-section against projectile energy of the reaction* $89_Y(p,pn)$ *for the experimental and calculated results.*

3.2. Comparisons of Theoretical Results with Experimental Values

To improve the reliability of available theoretical and experimental reaction cross-section data, the experimental and theoretical total cross-section results were compared using Pearson's correlation coefficient (R) [33, 34].

The theoretical excitation functions are plotted along with the experimental excitation functions against the projectile energies and are shown in Figures 1-5 and in Tables 1-5. The excitation function for the measured experimental value is represented by black line. The red line represents the calculation based on pre-equilibrium nuclear reaction while the green line represents the calculation based on the compound nuclear reaction. The results obtained were done by varying the level density and exciton number parameters of the reaction cross-sections [20].

$$R = \frac{\sum_{i=1}^{N}(X_{ti} - \langle X_t \rangle)(X_{ei} - \langle X_e \rangle)}{n-1(S_{X\,t})(S_{X\,e})}$$

Where, R-is correlation coefficient, $\langle X_t \rangle$ and $\langle X_e \rangle$ represent the mean theoretical and experimental cross-sections respectively, X_{ti} and X_{ei} are the theoretical and experimental cross-sections of the i^{th} value respectively, N is number of the theoretical and experimental data where as $S_{X\,t}$ and $S_{X\,e}$ are the standard deviation of the theoretical and experimental cross-sections respectively. Each mentioned variable represents the following mathematical relations:

$$\langle X_t \rangle = \frac{1}{N}\sum_{i=1}^{N}(X_{ti}) \; S_{Xt} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(X_{ti} - \langle X_t \rangle)}$$

$$\langle X_e \rangle = \frac{1}{N}\sum_{i=1}^{N}(X_{ei}) \; S_{Xe} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(X_{ei} - \langle X_e \rangle)}$$

The value of R is in between -1 and 1. Where, 1 is the total positive linear correlation, 0 is no linear correlation, and −1 is total negative linear correlation. If 0 < R < 0.3, the correlation is weak and positive, if 0.3 ≤ R < 0.7, it describes moderate correlation and for 0.7 ≤ R < 1, the correlation is strong and positive. The whole excitation functions of 89_Y isotopes are re-measured and compared with the recommended experimental data taken from EXFOR IAEA, library using Pearson's correlation coefficient.

4. Conclusion

Proton induced reactions on the target element yttrium isotope were studied upto 80 MeV. The excitation functions for five reactions of the type $89_Y(p,xn); x = 2-4, 89_Y(p,pxn); x = 1-2$ were studied using the computer code COMPLET. The newly calculated cross-section data of this study can help to clarify the relationship between the experimental data and the theoretical values. Cross section deduced from the production of $87{,}86_Z$ *and* 88_Y in most cases show a good continuation of the eventually existing measured experimental data in a lower energy region for the total exciton number $n_0 = 1\,(1p + 0h)$ and level density parameter ACN/10 of the excitation functions.

The experimental data were compared with those calculated values using the computer code COMPLET. The calculated values using code COMPLET were not systematic and gave only partly good estimations for several reactions. There are inconsistencies in the results between theory and experiment, especially in the multi-particle emission reactions. The evaporation peak broadens and inconsistencies develops with theoretical predictions.

The excitation functions for these calculations were constructed by using our new results combined with data from the EXFOR literature. The experimental and theoretical values were comparable for all the reaction channels considered in this study and were strongly correlated with the target isotope of yttrium.

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Conflicts of Interest

The authors declare no conflicts of interest.

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