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NUCLEAR REACTION CROSS-SECTION EVALUATION OF ISOTOPES OF SOME ELEMENTS AROUND 14 MeV USING EXIFON CODE

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ABSTRACT

EXIFON 2.0 code was used to calculate the (n, P) of ^{54}Fe, ^{56}Fe, ^{55}Mn, ^{58}Ni, ^{60}Ni, ^{27}Al, ^{50}Cr, and ^{239}Pu. Results of the evaluated excitation functions obtained with the code EXIFON were compared with the ENDF data retrieved from IAEA Nuclear Data section ENDF data library.The results of the evaluated excitation functions agree well with the ENDF data, especially for nuclides with EVEN-EVEN nucleus. The percentage deviation of total cross section from ENDF values obtained for this work is less than 1% for, ^{58}Ni, ^{50}Cr, ^{56}Fe, ^{55}Mn, ^{60}Ni, ^{27}Al and ^{239}Pu except for ^{54}Fewhich is1.81%while for the entire work the percentage deviation of the total cross section from ENDF values obtained is 0.24% . However, these results show good agreement with available measured data.

Keywords: Nuclear reaction, Cross-Section, EXIFON Code.

INTRODUCTION

The accurate knowledge of the cross-sections and the excitation functions of fast neutron reactions are of interest from the point of view of nuclear reaction theory, fission and fusion reactor technology, fast reactor design and control calculations, neutron fluency monitoring, safeguards, neutron therapy, Medical Physics, activation and prompt radiation analysis, radionuclides production and applications of data in dosimetry. Dose calculations are very important in nuclear medicine because of the amount of radioactivity required for specific diagnostics, therapeutic applica-tions and nuclear reactor applications. The cross section is calculated in terms of the effective area, which the nucleus presents to the beams of the bombarding particles (projectiles). It is measured in barns, (1 barn= 10^{-28} m^2).

$$\sigma = \frac{number\ of\ events\ of\ a\ given\ type\ per\ nucleus}{number\ of\ incident\ particles\ per\ unit\ time}$$

Nuclear reaction Cross section is one of the most important quantities encounter in nuclear reactions (Bauer *et al*., 1997). It can also be defined as the probability of interaction. Thus given a reaction of a given type, the cross section for that reaction is the probability that its reaction will take place or simply the probability of occurrence of the said reaction. There is cross section for absorption, for scattering and for fission (Kittern *et al*., 2009).

The sum of the cross sections due to absorption, scattering and luminescence that make up a given reaction is the total cross section. The cross-sections for various nuclear reactions depend on bombarding energy in a highly individualistic manner. The detailed dependence of cross-section on bombarding energy is often called the "excitation function "for the particular reaction (Ahmad *et al*., 2017).

The theories of the cross-section of nuclear reactions in which a compound nucleus is formed are divided into two broad classifications. At low bombarding energies, the excited levels of the compound nucleus are discrete and may be widely spaced. Here the reaction cross-sections are described by a resonance theory. At higher bombarding energies, the excited levels in the compound nucleus are more closely and partially overlapped. In this energy domain, the continuum theory describes the general variation of cross-section with bombarding energy (Ibrahim, 1995). The energy dependence of nuclear cross-sections, averaged over individual fluctuations and resonances, is expressed in terms of two parameters of the inner nuclear structure. Consider the case of incident neutrons. The two parameters are the nuclear radius R and the wave number K of the incident neutron after it is in the interior of the compound nucleus. The excitation functions of ^{58}Ni and ^{55}Fe reaction for energies up to 70 Mev as reported by Asres *et al.* (2019), indicated that the reaction cross-section mechanisms of ^{58}Ni isotopes induced by alpha particle may be obtained using computer code COMPLET. The cross sections for various nuclear reactions depend on bombarding energy in a highly individualistic manner. The detailed dependence of cross section on bombarding energy is often called the "excitation function" for the particular reaction (Robley, 1995). Excitation function is presented as graphical plots of cross-section against the energy of incident particle. In nuclear data analysis, it describes the probability that nuclear reactions can occur at particular energies of incident particle (Ahmad *et al.*, 2017). A nuclear reaction occurs when the waves of a nucleon or a nucleus interact with another nucleon or nucleus. Nuclear reactions are characterized by the incoming nuclei and the outgoing reaction products. Thus, after the reaction, the product nuclei which are the residual nucleus and the ejectile leave the point of contact in different directions (Ebiwonjumi, 2014). The cross section Evaluation Working Group (CSEWG) in 2001 discussed the need for more data evaluation as it is an international group that usually review nuclear Cross section data across the globe for work that is perform by either individual or group by either experiment or computer code.

THEORETICAL FRAMEWORK

EXIFON code is an analytical model, a statistical multi-step reaction model, capable of giving a unique description of emission spectra, angular distributions and activation cross section including equilibrium, pre-equilibrium as well as direct theory (collective and non-collective) processes (Kalka, 1992). The code is restricted to neutron-, proton-, and alpha-induced reactions with neutrons, protons and alphas, photons in the outgoing channels. Three basic ideas mainly influenced this step from simple compound nucleus models and single step direct models towards statistical multi-step theory. They include the classification of nuclear states by their complexity or exciton numbers as predicted by Griffin (1967), the distinction between bound and unbound state configuration as explained by Feshbach (Jonah, 2013) and the possibility of treating the chaotic nuclear Hamiltonian as a random matrix as presented by Agassi *et al.* (1975). These ideas were realized in many body theories by the Born series expansion of the related part of the mass operator in powers of the residual interaction with the latter replaced by random matrices.

Thus, expression for the differential cross section of the reaction (a,xb) after energy ensemble were obtained as (Kalka, 1991):

$$(a; xb) = (SMD) + (SMC) + (MPE) \quad (1)$$

SMD is the Statistical Multi-Step Direct Process, SMC is Statistical Multi-Step Compound Process, SMD + SMC is 1st chance emission process, MPE is Multi particle emission process calculated in a pure SMC concept. In these cases, we can account for neutron, proton and alpha induced reactions with neutron, protons, alphas and protons in the outgoing channels. In the statistical multi-step model, the total emission spectrum of the process (a; xb) given as d a; xb=dE is given in three main parts as (Kalka, 1991)

$$\frac{d\sigma_{a,xb}\,(E_a)}{dE_b} = \frac{d\sigma_{a,b}^{SMD}\,(E_a)}{dE_b} + \frac{d\sigma_{a,b}^{SMC}\,(E_a)}{dE_b} + \frac{d\sigma_{a,xb}^{MPE}\,(E_a)}{dE_b} \quad (2)$$

The first term on the right-hand side of equation (2) represents the statistical multistep direct (SMD) part which accounts for single-step to five-step contributions. The second term represents the statistical multistep compound (SMC) emission. SMD plus SMC represents the first chance emission process (Kalka, 1992). The last term represents the multiple particle emissions. These terms are summarized as:

$$\frac{d\sigma_{a,xb}^{MPE}\,(E_a)}{dE_b} = \sum_c \frac{d\sigma_{a,cb}\,(E_a)}{dE_b} + \sum_{c,d} \frac{d\sigma_{a,cbd}\,(E_a)}{dE_b} + \dots\dots \quad (3)$$

The EXIFON code predicts emission spectra, angular distribution and activation cross section considering equilibrium, pre-equilibrium and direct process and accounts for multiple particles of the compound system up to three decays. It also analyses reactions involving neutrons, protons and alpha particles with neutrons, protons, alpha and photons as emitted particles. It is limited to target nuclide of mass A>20 and incident energies below 100MeV (Kalka, 1991).

The statistical multistep reaction model employed in the EXIFON code was based on many-body theory (Green's Function Formalism). The code performs calculation by summing the contributions from statistical multistep direct (SMD), statistical multistep compound (SMC) and the multistep particle emission (MPE) processes. Consider the process (a, xb) in which a represents the projectile and b the emitted particle. Assume a=neutrons n, and b = neutrons n, protons p, alpha = α or gamma= γ. At incident energy E_a the optical model (OM) reaction cross section ${\sigma_a}^{OM}$ and the energy integrated partial cross-section satisfies the reaction:

$${\sigma_a}^{OM} = \sum_b \sigma_{a,b} \quad (4)$$

$$\sigma_{a,b} = \sum_c \sigma_{a,bc} \quad (5)$$

$$\sigma_{a,bc} = \sum_d \sigma_{a,bcd} \quad (6)$$

$$\text{where}\,\sigma_{a,b} = {\sigma_{a,b}}^{SMC} + {\sigma_{a,b}}^{SMD} \quad (7)$$

Equation (7) represents the total first chance emission. $\sigma_{a,b^{SMC}}$ is the statistical multistep compound reaction cross-section and $\sigma_{a,b^{SMD}}$ is the statistical multistep direct reaction cross section. The relations between the optical model (OM) and cross section and the energy integrated partial cross section is satisfied at each energy incident (E_a).

$$\sigma_a^{OM} = \sum_b \sigma_{a,b} \quad (8)$$

$$\sigma_{a,b} = \sum_c \sigma_{a,cb} \text{ and } \sigma_{a,cb} = \sum_c \sigma_{a,cbd} \quad (9)$$

$$\sigma_{a,b\gamma} = \sigma_{a,b} - \sum_{c\neq\gamma} \sigma_{a,bc} \quad (10)$$

$$\sigma_{a,bc\gamma} = \sigma_{a,cb} - \sum_{d\neq\gamma} \sigma_{a,bcd} \quad (11)$$

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

A unique description (a, xb) emission spectra where $a, b = n, p, \propto$ and γ (Neutron, Proton, Alpha and Gamma-ray) as well as excitation function (activation) (Kalka, 1991).Statistical Multi-step Compound (SMC) Cross Section. The SMC Cross Section has the form $(b = n, p, \propto, \gamma)$.

$$\frac{d\sigma^{SMC}(E_a)}{dE_b} = \sigma^{SMC}(E_a) \sum_{N=NO} \frac{\tau_N(E)}{\hbar} \Gamma_{Nb}(E, E_b) \uparrow \quad (12)$$

Where $\tau_N(E)$ satisfies the time-integrated master equation,

$$-\hbar\, \delta_{NN_0} = \Gamma_{N-2}^{(+)}(E) \downarrow \tau_{N-2}(E) \Gamma_{N+2}^{(-)}(E) \downarrow \tau_{N+2}(E) - \Gamma_N(E)\tau_N(E), \quad (13)$$

The EXIFON code installed on a personal computer has time for one full-scale description per nucleus (which includes all activation cross-section plus emission spectra from zero up to 100 MeV incident energy) which strongly depends on the incident energy (Kalka, 1991). The excitation functions are evaluated from a plot of cross section against energy. The values of the cross section are given in barns, while that of energies is in MeV. The input and output directory are first defined, then the target nucleus specified. The incident particle (in this case Neutron) selected followed by selecting the excitation function in the general option section for this calculation. The number of incident energy is specified, then the first incident energy (in MeV), and then the incident energy step (in MeV). In modification, the shell structure effect is selected. The option with shell effect is selected for each target nucleus. An output data (OUTEXI) for the calculation is then stored in the output directory. In addition, the DAT file name A2N, ALF, and AP (for Neutron-2-Neutron, Neutron-Alpha, and Neutron-Proton reaction respectively) are stored in the set output directory. Secondly, the option without shell effect is selected for each target nucleus. An output data (OUTEXI) for the calculation is stored in the set output directory. The DAT file name A2N, ALF, and AP (for Neutron-2Neutrons, Neutron-Alpha, and Neutron-Proton reaction respectively) are stored in the set output directory. The data in the DAT files are then plotted as chats or graphs or viewed using a DAT file Viewer.

RESULTS AND DISCUSSION

The results of the excitation function evaluated of ^{54}Fe, ^{56}Fe, ^{55}Mn, ^{58}Ni, ^{60}Ni, ^{27}Al, ^{50}Cr, and ^{239}Pu are plotted with ENDF data.

1. Total Cross Section against Energy for ^{54}Fe (n, p) ^{54}Mn

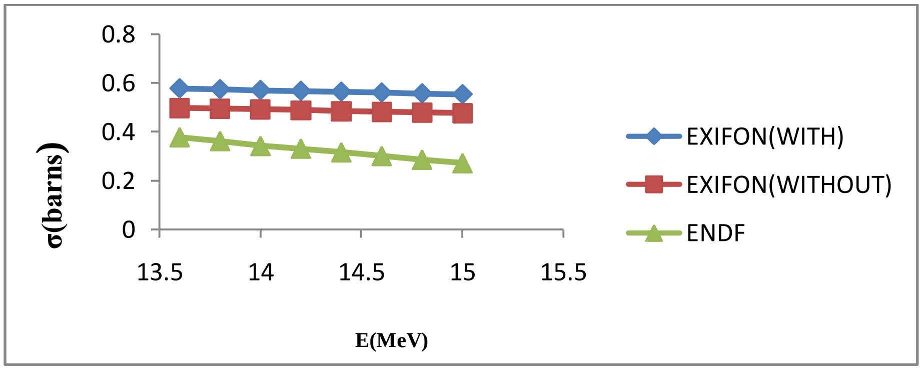

Figure 1: Fe-54(n, p) Reaction

2. Total Cross Section against Energy for ^{56}Fe (n, p) ^{56}Mn

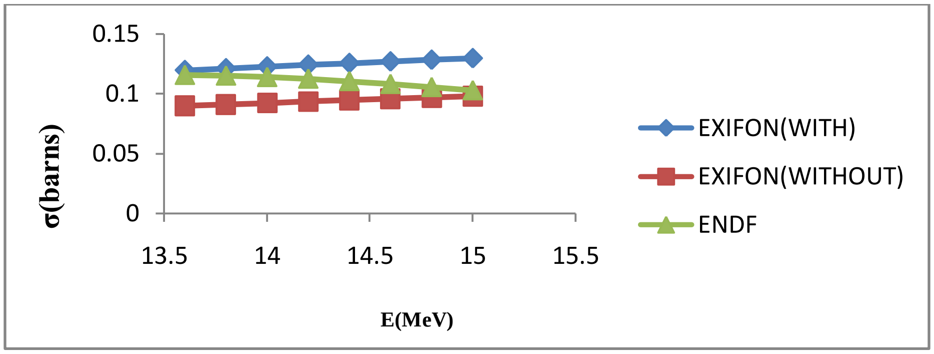

Figure 2: Fe-56(n, p) Reaction

The values obtained from $Exifon_w$ and $Exifon_{wo}$ shows a good agreement with a significant difference of 0.0801, 0.0797, 0.0793, 0.0789, 0.0784, 0.078, 0.077 and 0.0771 at Energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, and 15.0 respectively. The trend shows a good agreement before it deviates; the values of the $Exifon_{wo}$ and ENDF have significant differences of 0.1202, 0.1326, 0.145, 0.1572, 0.1693, 0.1813, 0.1932 and 0.02043 at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 respectively. The mean deviation of $Exifon_{wo}$ and ENDF is 0.0181.

The $Exifon_w$ and $Exifon_{wo}$ shows an agreement with each other in there trend, but $Exifon_w$ shows a very good agreement with the retrieved data at energy of 13.6 MeV to 14 MeV before it deviates and later shows a very good agreement from 14.6MeV to 15MeV with $Exifon_{wo.}$ The difference obtained between $Exifon_w$ and $Exifon_{wo}$ at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0298, 0.03, 0.0304, 0.0307, 0.0309, 0.0311, 0.0314 and 0.0316 respectively while the difference between $Exifon_w$ and ENDF from the values obtained at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0038, 0.0058, 0.0086, 0.0115, 0.0149, 0.0186, 0.0226 and 0.0266 respectively. The deviation of $Exifon_w$ and $Exifon_{wo}$ is 0.0307 while the mean deviation of $Exifon_w$ and ENDF is -0.00005. The cross section for with and without shell effects increases with increase in energy but the ENDF data decreases with increase in energy.

3. Total Cross Section against Energy for ^{55}Mn (n, p) ^{55}Cr

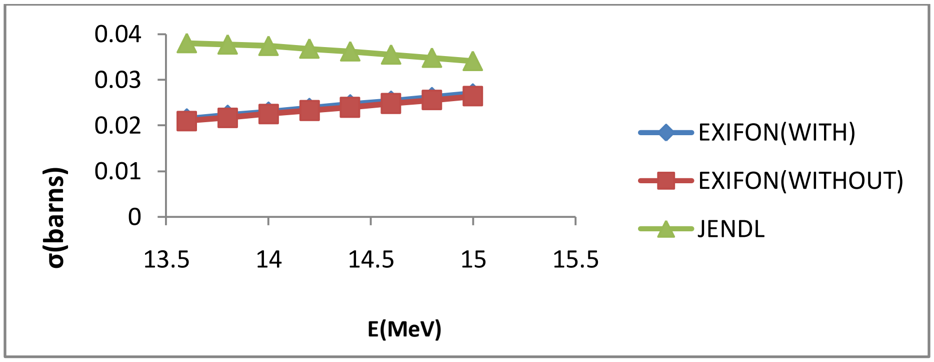

Figure 3: Mn-55(n, p) Reaction

4. Total Cross Section against Energy for ^{58}Ni (n, p) ^{58}Co

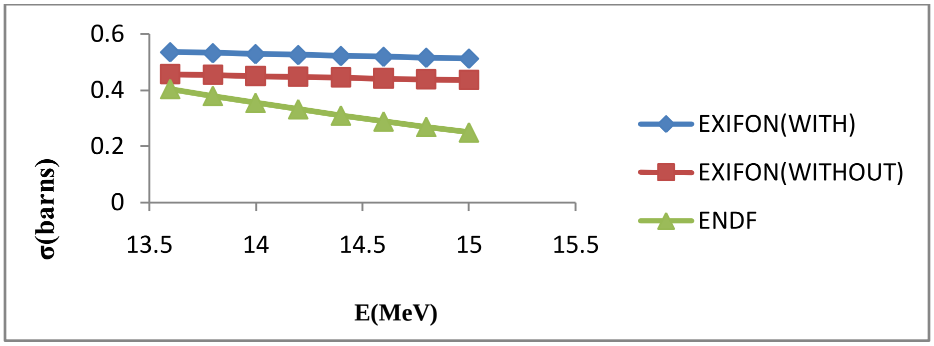

Figure 4: Ni-58(n, p) Reaction

5. Total Cross Section against Energy for ^{60}Ni (n, p) ^{60}Co

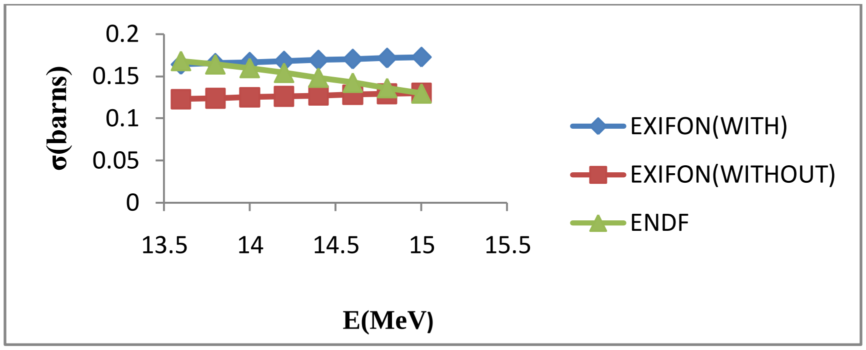

Figure 5: Ni-60(n, p) Reaction

The values obtained using Exifon$_w$ and Exifon$_{wo}$ are in very good agreement with each other and show disagreement at energy 13.6 to 14.0 before moving on the same trend up to energy 15.0. The difference in the value obtained from JENDL and Exifon at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0165, 0.0154, 0.0145, 0.013, 0.0116, 0.0101, 0.0086 and 0.0071 respectively. The mean deviation is 0.00039.

The values obtained Exifon$_w$ and Exifon$_{wo}$ shows an agreement with each other. The Exifon$_{wo}$ show a good agreement with the retrieved data at energy of 13.6MeV to 14.2MeV before it deviates. The values obtained from Exifon$_{wo}$ and Exifon$_w$ at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0785, 0.0781, 0.0777, 0.0773, 0.0769, 0.0769, 0.0764, and 0.0761 respectively while the difference between Exifon$_{wo}$ and ENDF is 0.0529, 0.0744, 0.096, 0.1154, 0.1349, 0.1528, 0.1694 and 0.1859 at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0. The average deviation between Exifon$_{wo}$ and Exifon$_w$ is 0.0772 while the mean deviation for Exifon$_{wo}$ and ENDF is 0.000875.

The values obtained with Exifon$_w$ and Exifon$_{wo}$ shows agreement with their trend. The values obtained with Exifon$_w$ and ENDF show good agreement at energy 13.6 MeV to 14.2 MeV before it deviate later show good agreement with Exifon$_{wo}$ at energy 14.4 MeV to 15 MeV. The difference between Exifon$_w$ and Exifon$_{wo}$ at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0416, 0.0414, 0.0416, 0.0418, 0.142, 0.0421, 0.0424, and 0.0425 respectively while that of Exifon$_{wo}$ and ENDF at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0043(ENDF higher), 0.0001, 0.0067, 0.0137, 0.0206, 0.0278, 0.0353, and 0.0428 respectively. The average deviation of Exifon$_w$ and Exifon$_{wo}$ is 0.0419 while the mean deviation of ENDF and Exifon$_{wo}$ is 0.000012.

6. Total Cross Section against Energy for ^{27}Al (n, p) ^{27}Mg

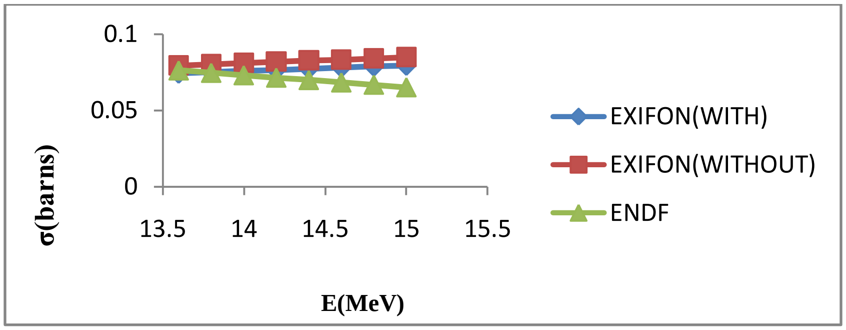

Figure 6: Al-27(n, p) Reaction

7. Total Cross Section against Energy for ^{50}Cr (n, p) ^{50}V

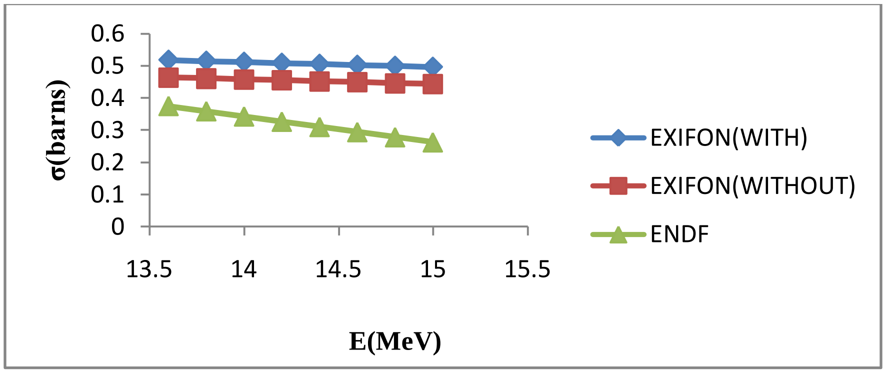

Figure 7: Cr-50(n, p) Reaction

8. Total Cross Section against Energy for ^{239}Pu (n, p) ^{239}Np

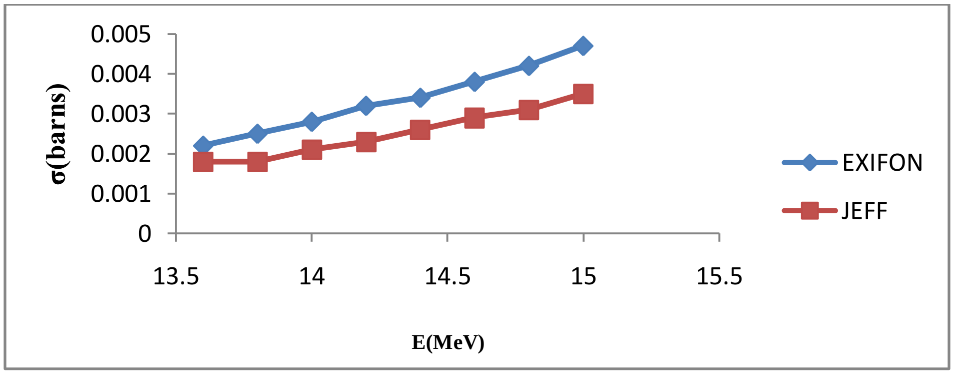

Figure 8: Pu-239(n, p) Reaction

The values obtained from Al-27 with $Exifon_w$ and $Exifon_{wo}$ shows a good agreement with the ENDF data at energy 13.6 MeV to 14.5 MeV before it deviates. The difference between $Exifon_w$ and $Exifon_{wo}$ at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0052, 0.0052, 0.0053, 0.0054, 0.0055, 0.0054, 0.0055, and 0.0056 respectively while that for $Exifon_{wo}$ and ENDF at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0021(ENDF higher), 0.0003, 0.0027, 0.005, 0.0073, 0.0097, 0.0119 and 0.0141 respectively. The average deviation between $Exifon_{wo}$ and $Exifon_w$ is 0.0054 while mean deviation for $Exifon_w$ and ENDF is 0.0000375.

The $Exifon_w$ and $Exifon_{wo}$ show good agreement and are consistent within the used energy range. Both the $Exifon_w$ and $Exifon_{wo}$ are in agreement with the ENDF in their trend and from energy 13.6 to 14.4 before a deviation. The difference between $Exifon_w$ and $Exifon_{wo}$ at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.055, 0.0548, 0.0544, 0.0542, 0.0538, 0.0535, 0.0531, and 0.0528 respectively while that for $Exifon_{wo}$ and ENDF at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8, 15.0 are 0.0877, 0.1011, 0.1145, 0.1279, 0.1414, 0.1546, 0.1676 and 0.1807 respectively. The average deviation between $Exifon_w$ and $Exifon_{wo}$ is 0.0539 while the mean deviation for $Exifon_{w0}$ and ENDF is 0.0000375 The values with Exifon has the same trend with JEFF and are also in trend even though with a difference of 0.0004, 0.0007, 0.0017, 0.0009, 0.0008, 0.0007, 0.0011 and 0.0012 at energy 13.6, 13.8, 14.0, 14.2, 14.4, 14.6, 14.8 and 15.0 respectively. The mean deviation is 0.0000375.

General Deduction

These results show the stability and nature, which is either ODD-EVEN, EVEN-ODD or EVEN-EVEN. The mass of the nucleus affects the nuclear reaction cross-section and also determines whether it decreases or increases. The trend of all the isotopes of interest in this work were decreasing as the energy increases except Pu-239 in which the nuclear reaction cross-section increased because it is a heavy nuclide. EVEN-EVEN nuclides are more stable than EVEN-ODD and ODD-EVEN because of their stability nature. Chromium has very low level density and a propensity for low-lying unnatural parity states. The low level density manifests itself as non-statistical fluctuation of neutron cross section at low energies.

CONCLUSION

The excitation function was calculated based on a theoretical model code EXIFON. EXIFON adequately account for the interaction of nucleus with neutron in the energy range of interest. Data of the excitation function were compared with measured data from ENDF, JENDL and JEFF Data library. EXIFON can predict the cross section data where experimental and evaluated data is scanty. Although there were little deviations in some of the nuclides of interest, the trend showed that EXIFON can actually produce an improved data where data is not available or fail to fulfill the required accuracy. The EXIFON code adequately matches the ENDF data for the (n, p) reaction.

REFERENCES

Agassi, K., H. A. Weidenmulter & G. Mantzouranis, (1975).Generalized Exciton Model for the Description of Preequilibrium Processes, *Phy. Rep*. 22 (1975) 145.

Ahmad, I. Koki, F. (2017).Calculation of Reactions of Cross Section for Neutron-Induced Reactions on ^{127}I Isotope. *International Journal of Medical Physics, Clinical Engineering and Radiation Oncology*, 6, 344-359.Doi: 10.4236/ijmpcero.2017.63031.

Bauer, R W, Anderson, J D, Grimes, S M, and Madsen, V A. (1997).Application of simple ramsauer model to neutron total cross sections. United States: N. P., 19.

Charles Dunford (2001). Cross Section Evaluation Working Group. Brook Haven National Laboratory Upton, New York 11973-5000.

Dauda Aliyu (2011) Nuclear Model Calculation of Excitation Functions of Neutron Induced Reactions on Structural Materials of the Miniature Neutron Source Reactor.

Ebiwonjumi, Y.E.C.B.F. (2014). Determination of Nuclear Reaction Cross-Section for Neutron-Induced Reactions in Some Odd-A Nuclides. Advanced in Physics Theories and Applications, 32, 55-69.

Griffin, J.J. (1967). A Unique Classification of Nuclear States, Phy. Lett.248, 5.

Ibrahim A.S (1995) (n, p) and(n,$\propto$) Reactions Cross-Section Measurement and Systematic Around 14Mev Neutron Energy.

Jonah S.A. And Agu M.N (2013). Workshop on Nuclear Reaction Theory and Cross Section Data Determination using Computer Codes.

Kalka, H. (1991). EXIFON – A Statistical Multi-step Reaction Code, Report, Technische Universitat Dresden, Germany.

Kalka, H. (1992) Hadrons and Nuclei Statistical Multistep Reaction from 1 to 100MeV. Zeitschrift Physik a Hadron and Nuclei, 299, 289-299.

Kettern, K., H. H. Coenen, and S. M. Ã. Qaim. (2009). Quantification of Radiation Dose from Short-lived positron emitters formed in human tissue under proton therapy conditions, Vol. 78, pp. 380-385.

Kettern, K., H. H. Coenen, and S. M. Ã. Qaim (2009). Quantification of Radiation Dose from Short-lived positron emitters formed in human tissue under proton therapy conditions,Vol. 78, pp. 380-385.

Muhammed, K., Onimisi, M.Y., Jonah, S.A., (2011): Investigation of the Shell Effect on Neutron Induced Cross-Section of Actinides. *Journal of Nuclear and Particle Physics* 1(1), 6-9.

Robley D. E, (1995).Atomic Nucleus. Massachusetts Institute of Technology, p. 441.

Rubbia C. (1994) Conceptual Design of a fast Neutron Operated High Power Energy Amplifier. CERN/AT/95-44 (ET). American Institute of Physics Conference Proceedings 346, International Conference on Accelerator-Driven Transmutation Technologies and Applications, Las Vegas.

Yehuwdah E.C, Bamidele F. Ebiwonjumi (2014). Determination of Nuclear Reaction Cross-Section for Neutron – Induced Reactions in some odd-A Nuclides.

YihunieHibstie Asres1, Manny Mathuthu and YinagerAschalewFerede (2019).Investigation of Nuclear Reaction Mechanisms of Nickel Isotopes at Various Energies Induced by Alpha Particles. J. Phys. Commun.