Fluorine production and its role in cancer diagnosis

$^{15}N(\alpha,n)^{18}F$ and $^{18}F(n,\alpha)^{15}N$

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Abstract. Fluorine-18, a radioactive isotope, is extensively utilized in medical applications, particularly for cancer diagnosis. This study investigates the production and reaction mechanisms of Fluorine-18 through the calculation of cross-sections for the reaction $^{15}N(\alpha, n)^{18}F$. The notable electronegativity of Fluorine, which arises from the configuration of its five electrons in the outer 2p shell, underlines its remarkable capacity to attract electrons, thereby emphasizing its chemical significance. Additionally, the cross-sections for the reverse reaction, $^{18}F(n, \alpha)^{15}N$, were analyzed to further comprehend its behavior under specific conditions. The results of this investigation demonstrate that the highest probability of producing Fluorine-18 occurs within the energy range of 8.7 to 15 MeV, divided into 0.15 MeV increments. The threshold energy requisite for initiating this reaction is precisely determined to be 1.05117 MeV. Moreover, semi-empirical equations defining the cross-sections for the reverse reaction were deduced. These equations incorporate critical parameters, including the masses of the incident and outgoing particles, the target nucleus and resulting daughter nucleus, as well as the spin and parity of the participated nuclei. Detailed analysis indicates that the peak probability for the reverse reaction, $^{18}F(n, \alpha)^{15}N$, is achieved at an energy level of 16.3444 MeV when the incident neutron energy is approximately 9.3736 MeV. Across varying neutron energy levels, the corresponding cross-sections exhibit distinct fluctuations characterized by multiple peaks. Specifically, at an incident neutron energy of 11.3736 MeV, a maximum cross-section value of 8.2743 millibarns (mb) is observed. For neutron energies resulting from the reverse reaction, cross-sections span values ranging from 16.3444 mbarn to 0.4879 mbarn as the associated energy decreases from 11.6236 MeV to 6.3738 MeV. This comprehensive dataset provides critical insights into understanding and optimizing Fluorine-18 production for medical applications.

Key words: reverse reaction , cross section , fluorine , Semi-empirical , medical field .

INTRODUCTION

When two charged nuclei manage to overcome their Coulomb repulsion, their internal components may undergo a rearrangement. This process is comparable to the reorganization of atoms during a chemical reaction, but in this case, it leads to a nuclear reaction. Typically, these reactions occur when a target nucleus is bombarded with a nuclear projectile, often a nucleon (neutron or proton) or a lightweight nucleus like a deuteron or an α-particle [1]. At relatively low excitation energies (below 10 MeV), most nuclear reactions result in the formation of two nuclei, one of which has a charge and mass number nearly identical to that of the target nucleus. Such reactions can be represented by specific types of equations :

$$X + a \rightarrow Y + b \tag{1}$$

The Q– value of the reaction is defined as the difference between the final and initial kinetic energies:

$$Q = Tb + Ty - Ta \tag{2}$$

$$Q = [Ma + Mx - Mb - My] C^2 \tag{3}$$

If Q is positive , the reaction is said to be an exo-ergic process; if Q is negative, it is endo-ergic process [1]. So, the Q < 0 process cannot occur spontaneously, which means that there is a threshold energy $Ta_{(thr)}$ given by [1]:

$$Ta_{(thr)} = E_{thr} = -Q\,(1 + Ma/Mx) \quad (4)$$

The reaction cross section is a physical term calculated through a specific area. The larger the area, the higher the likelihood of the reaction occurring. [5,6]. The cross section, a unit of area, is used to calculate the cross section of a nuclear reaction, as its incidence is within the square of the nuclear radius, since barn = 10-24 cm^2, Bombardment of particles causes multiple reactions, producing various elements. The cross section of reaction products and the entire reaction cross section are calculated through the relationship [7]:

$$\sigma_{tot} = \Sigma i\, \sigma i \quad (5)$$

The cross section of each reaction within the main reaction is denoted by σi.

The kinetic energies of the reaction products can be used to study any specific reaction. Devices designed for sensing radiation and particles classify their energy. Cross-section calculations are crucial for obtaining basic and essential information [8]. Quantum mechanics can be utilized to calculate the cross section of any reaction by utilizing mathematical models of nuclei. The expected and observed values of different cross sections can be calculated and compared. The nuclear models' hypotheses can be confirmed [8]. The cross-section provides a description of the interaction between particles and the substance as defined above.

The cross-section is the probability of a specific nuclear reaction occurring by determining the actual size of the nucleus. [3], The study of cross-sections of reactions is a crucial aspect of understanding Nuclear Systems [4]:

$$\sigma = R / I \quad (6)$$

The cross section of the nuclear reaction is denoted by σ. The number of interactions per unit time is denoted by R.

RECIPROCITY THEOREM

The cross sections A (α, n) B can be measured as a function of kinetic energy Kα (Kα = Kinetic energy of α-particle) [9, 10]. The reciprocity theorem is used to calculate cross sections B (n, α) A for the reverse reaction based on the kinetic energy of neutrons. K_n (K_n = Kinetic energy of neutrons) [11]. The reciprocity theorem is based on a specific relationship

$$\sigma_{(\mathbf{n},\boldsymbol{\alpha})} = {g_{\mathbf{n},\boldsymbol{\alpha}} M_{\boldsymbol{\alpha}}\; T_{\boldsymbol{\alpha}}} \Big/ {g_{\boldsymbol{\alpha},\mathbf{n}} M_{\mathbf{n}}\; T_{\mathbf{n}}} \quad \sigma_{(\alpha,n)} \quad (7)$$

The cross-sections of (α, n) and (n, α) reactions are represented by σ (α, n) and σ (n, α, respectively.

g is a statistical factor.

Δ is the De–Broglie Wave Length divided by 2π and is given by:

$$\lambda\!\!\!^{-} = \hbar / MV \quad (8)$$

Here, ħ represents the Dirac constant (h / 2π), where h is the Planck constant. M and V denote the mass and velocity of either an α particle or an n particle, respectively. The statistical g-factors are defined as follows:

$$g_{\alpha,n} = \frac{2Jc + 1}{(2IA + 1)(2I\alpha + 1)} \quad (9)$$

$$g_{\alpha,n} = \frac{2Jc + 1}{(2IA + 1)(2I\alpha + 1)} \quad (10)$$

The principle of conservation of momentum and parity necessitates that [11]: $I_A + I_\alpha = J_c = I_B + I_n$

$$\pi A\,.\,\pi\alpha\,(-1)\ell\alpha = \pi c = \pi B\,.\,\pi n\,(-1)\,\ell n \quad (11)$$

The total angular momentum (Jc) and parity (πc) of the compound nucleus represent fundamental parameters that must be carefully evaluated. Similarly, the total angular momentum (IA) and parity (πA) of nucleus A are equally significant factors warranting attention. I_B and π_B The total angular momentum and parity of nucleus B are crucial factors to consider. I_α and π_α The total angular momentum and parity of the α-particle are crucial factors to consider. I_n and π_n The total angular momentum and parity of a neutron are crucial factors to consider.

Fluorine-18 is the most commonly utilized isotope in positron emission tomography scans. The isotope is a fluorescent one with a half-life of approximately 110 minutes. This isotope is highly beneficial due to its extended half-life and its emission of positrons with the lowest energy [1], The process of obtaining high-resolution images is significantly facilitated by this. Positron Emission Tomography PET is crucial in tutor diagnosis and staging due to its ability to provide functional information synchronized with anatomical details when combined with computed tomography (CT). Fluoride-18-Fluoride is a valuable PET tracer for pure radiotracers, as it is sub hydroxylated in bone crystals by fluorapatite, enhancing diffusion rates [2].

PET scans reveal an increase in 18-fluoride levels in bone lesions, indicating a boost in bone and blood growth. A PET scan using 18F-FDG labelled the brain, kidneys, bladder, and FDG breakdown, revealing radioactive urine and a large colon cancer tumour mass in the liver. PET is a crucial medical and research tool in imaging tumours, detecting metastases, and diagnosing diffuse brain diseases. It enhances understanding of the human brain, heart function, and supports drug development, and is used in pre-clinical studies.

RESULTS AND DISCUSSIONS

In Table No. 1, the cross sections of an incidental alpha particle with an energy ranging between 8.7 and 15 MeV are 0.9017-6.219 mbarn, respectively, and the values of the cross sections fluctuate according to the incident energy of the alpha particle, as shown in Figure 1. We note that the highest value for the probability of a nuclear reaction occurring when the alpha energy is 12.3 MeV is 9.3934 mbarn, as this is the best energy for producing an isotope of fluorine from the reaction of nitrogen-15 with the alpha particle, which is used in the medical field to diagnose cancer tumors using a PET camera.

The cross-section of the reaction $^{18}F\ (n, \alpha)^{15}N$ was calculated using the opposite reaction equation No. 3, based on the values of spin and parity for each of the reactants, products, and the complex nucleus, and these values were subjected to testing according to the above-mentioned equations No. The kinetic energy of the neutron was also calculated by calculating the interaction energy values Q_o (-0.8295 MeV) and calculating the threshold energy E_{th} (1.051174 MeV) based on the masses of the isotopes taken from.

The neutron energy values obtained from the reverse reaction of $^{18}F(n,\alpha)^{15}N$, as summarized in Table 1, indicate that the cross-sections range from 16.3444 mbarn to 0.4879 mbarn, while the corresponding energy span falls between 11.6236 MeV and 6.3738 MeV. Notably, the highest probability for the reaction occurs with a cross-section of 16.3444 mbarn when the neutron energy decreases to 9.3736 MeV, as illustrated in Figure 2. It is further observed that the cross-section values exhibit fluctuations with multiple peaks, including one at an incident neutron energy of 11.3736 MeV, where the cross-section reaches 8.2743 mbarn.

TABLE 1. Cross section as a function of energies alpha and neutron of $^{15}N(\alpha,n)^{18}F$,$^{18}F(n,\alpha)^{15}N$ reactions

Alpha energy (MeV)	X-Sections (mbarn)	Neutron energy (MeV)	X-Sections (mbarn)	Alpha energy (MeV)	X-Sections (mbarn)	Neutron energy (MeV)	X-Sections (mbarn)
8.7	0.9017	6.3738	1.5689	12	0.6068	9.1237	1.0557
8.85	3.7257	6.4988	6.4826	12.15	2.002	9.2487	3.4834
9	2.5745	6.6238	4.4796	12.3	9.3934	9.3736	16.3444
9.15	2.2636	6.7488	3.9386	12.45	4.99	9.4986	8.6825
9.3	1.3041	6.8737	2.2691	12.6	2.5275	9.6236	4.3977
9.45	2.0072	6.9987	3.4926	12.75	1.8976	9.7486	3.3018
9.6	0.8918	7.1237	1.5516	12.9	1.8034	9.8736	3.1379
9.75	0.4525	7.2487	0.7874	13.05	2.0545	9.9986	3.5749
9.9	0.3416	7.3737	0.5945	13.2	2.7135	10.1236	4.7215
10.05	0.2804	7.4987	0.4879	13.35	3.9134	10.2486	6.8093
10.2	0.36	7.6237	0.6263	13.5	5.1728	10.3736	9.0005

10.35	3.5059	7.7487	6.1002	13.65	4.9877	10.4986	8.6785
10.5	1.0813	7.8737	1.8814	13.8	3.6809	10.6236	6.4047
10.65	0.8968	7.9987	1.5604	13.95	2.6359	10.7486	4.5864
10.8	1.3011	8.1237	2.2639	14.1	2.1037	10.8736	3.6604
10.95	2.5425	8.2487	4.4239	14.25	1.9465	10.9986	3.3869
11.1	4.031	8.3737	7.0139	14.4	2.1529	11.1236	3.7459
11.25	3.0643	8.4987	5.3318	14.55	2.9228	11.2486	5.0857
11.4	1.9911	8.6237	3.4644	14.7	4.7554	11.3736	8.2743
11.55	1.9007	8.7487	3.3073	14.85	7.1782	11.4986	12.49
11.7	4.2841	8.8737	7.4543	15	6.219	11.6236	10.821
11.85	3.8527	8.9987	6.7036	------	------	------	------

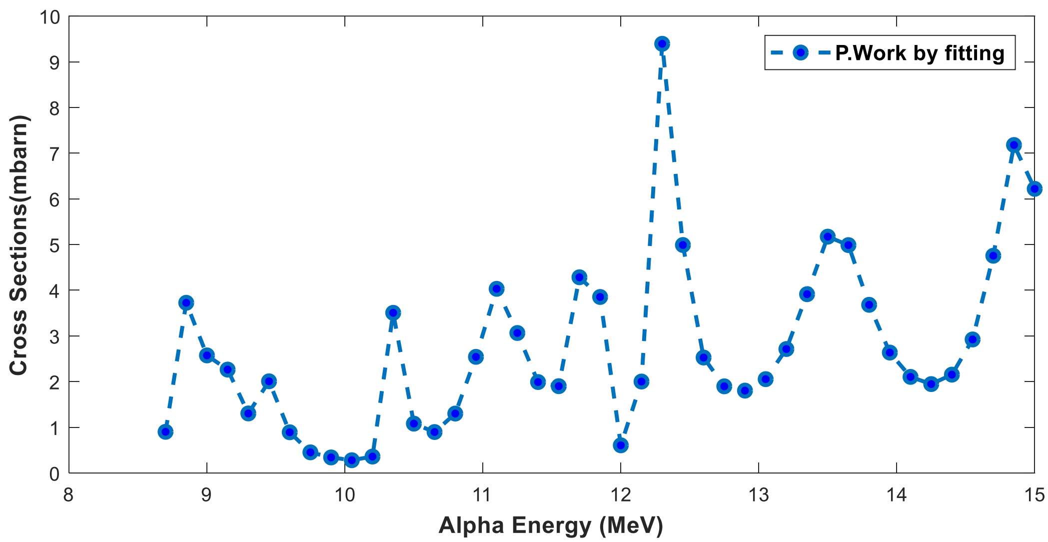

FIGURE 1. Cross Sections as a faction of alpha energy of $^{15}N\ (\alpha, n)^{18}F$

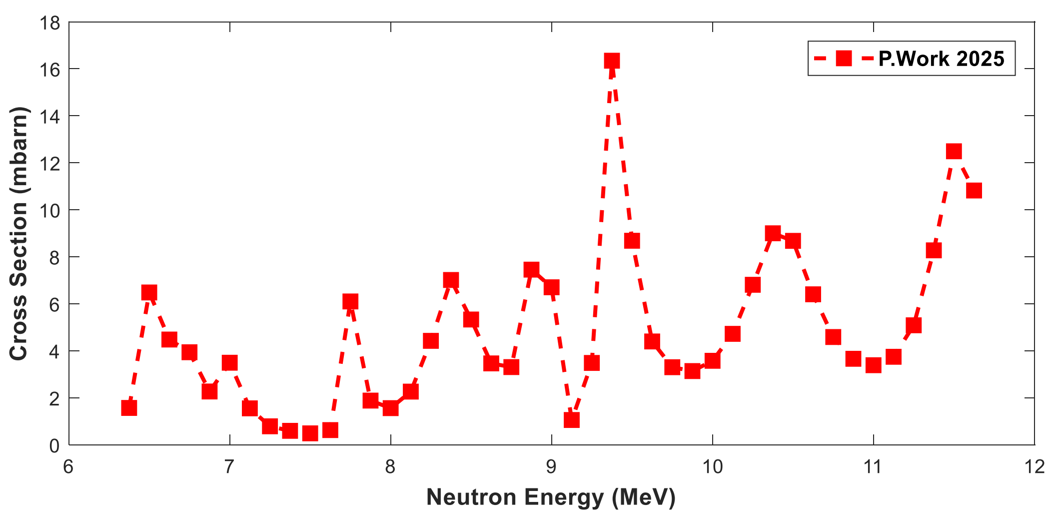

FIGURE 2. Cross Sections as a faction of neutron energy for $^{18}F\ (n, \alpha)^{15}N$

CONCLUSIONS

In reaction $^{15}N(\alpha, n)^{18}F$, it is clear from Figure 1 that the cross-section values fluctuate with the incidental alpha energy over the range 8.7-15 MeV, and that the highest probability of the reaction occurring and producing the fluorine isotope is 12.3 MeV is 9.3934 mb. The cross-section values are approximately constant for some values of the incident alpha energies. The highest probability of the reaction occurring and producing the nitrogen isotope from the reverse reaction $^{18}F(n,\alpha)^{15}N$ occurs when the energy of the incident neutron is 9.3736 MeV. The pattern of the relationship is oscillatory, while the remaining cross-section values fluctuate, and some of them are constant for some values of the incident neutron energy. In the reaction $^{15}N(\alpha, n)^{18}F$, it is clear from Figure 1 that the cross-section values fluctuate with the energy of the incident alpha over the range of 8.7-15 MeV. The highest probability for the reaction to occur and produce fluorine isotope is 12.3 MeV (9.3934 mb). The cross sections are almost constant for some values of the incident alpha energies. The reaction to produce the nitrogen isotope from the reverse process 18F (n, α)15N is most likely to occur when the incident neutron energy reaches 9.3736 MeV, corresponding to a cross-section of 16.3444 mb. The relationship exhibits an oscillatory pattern, with the remaining cross-sections showing fluctuations, and some remain constant at specific values of the incident neutron energy.

ACKNOWLEDGMENTS

This study was supported by Karabuk University Scientific Research Projects Coordination Unit. Project Number: KBÜBAP-24-YL-161.

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