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Study of Properties for Ca (a, n)Ti Reactions and n-Yield for Ca Isotopes (A=41-50)

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Abstract:

In this study, (⁴⁴Ti – ⁵³Ti) isotopes for one of intermediate elements (A>40) from Ca (α , n)Ti reactions with alpha energy from (10 to 50) MeV are used according to the available data of reaction cross sections obtained from Lab (TENDL-2012). The more recent cross sections data of Ca (α , n)Ti reaction is reproduced in fine steps of (0.5MeV), by using (MATLAB R2008b) program. These cross sections together with the stopping powers which calculated from the Zeigler formula by using SRIM-2013 have been used to calculate the n-yield for reaction by depend on Ca isotopes (⁴¹Ca – ⁵⁰Ca) as targets, and then clarify the behavior between the energies which corresponding to these cross sections and neutron yield for isotopes, and then we drowned the relationship between the n-yield for these equations and these energies. Was obtained on mathematical formulas and find constants those equations and these equations were calculated binding energy and reduced mass and also were calculated Q- value and threshold energy for each reaction and the relative abundance of the isotopes of entering and leaving for alpha reactions. And then drawing scheduled and discusses the results.

Keyword: Binding energy, Cross-Section, Neutron Yield, stopping power, Asymmetry and empirical formula.

1-Introduction

The (α , n) gneutron sources with intermediate mass nuclei as a target, it has the high neutron yield. Due to many advantages of the (α ,n)neutron source, such as their simplicity of installation, operation and low price compared to nuclear reactors, these neutron sources are used in activation analysis [1,2,3], calibration source [4], and industrial applications [5].

The binding energy can be calculated as the reduction in mass multiplied by the square of the velocity of light ($c^2 = 931.494013 \text{ MeV/u}$) [6]:

Where (Z and N) are the number of protons and neutrons, (M_H , M_n and $^A_Z M$) are three masses of hydrogen atom, neutrons and nucleus respectively.

 μ is the reduced mass calculated from the following equation [7]:

Where (m1) and (m2) are the atomic masses of the projectile and target nucleus, respectively.

The Q – value of the reaction $X(\alpha,n)Y$, is defined as the difference between the initial and final rest mass energies [7]:

Where (M_x, M_α, M_Y) and M_n represents the atomic masses of the target, incident particles, product nucleus and outgoing particle, respectively. From conservation law of energy [7].

The Q- value is positive, Q > 0, the reaction is said to be (excergic) or (exothermic).

When Q- value is negative, Q < 0, the reaction is (endoergic) or (endothermic). For (exoergic) reactions, threshold energy is (zero) and for (endoergic) reactions, the threshold energy is given by [8]:

$$E_{thr} = -Q_0 (1 + \frac{Ma}{Mx})$$
(4)

 $S_n = 931.5 [M_y + M_n - M_x]$ (5)

Where S_n is separation energies of neutron [7].

2- Cross section of the nuclear reaction

To characterize the probability that a certain nuclear reaction will take place, it is customary to define an effective size of the nucleus for that reaction, called a cross section [7]. The reaction cross section data provides information of fundamental importance in the study of nuclear systems. The cross section is defined by [9]:

Were R is the number of reactions per unit time per nucleus. I is the number of incident particles per unit time per unit area,

The cross section has the units of area and is of the order of the square of nuclear radius. A commonly used unit is the barn: $(1 \text{ barn} = 10^{-24} \text{ cm}^2)$

In general, a given bombarding particle and target can react in a variety of ways producing a variety of light reaction products per unit time. The total cross section is then defined as [10]:

$$\sigma_{tot} = \sum_{i} \sigma_{i} \qquad \dots \qquad (7)$$

Where σ_i is the partial cross section for the process.

3-Asymmetry energy:

The nuclear asymmetry energy, which is defined as the difference in energy per nucleon between the pure neutron matter and the symmetric nuclear matter, Asymmetry energy expresses the trend to particular stability of nuclei with N = Z for small A. Light nuclei become less stable if |N - Z| increases[7]. If we were to add more neutrons, they will have to be more energetic, thus increasing the total energy of the nucleus, so that it is more favorable to have an approximately equal number of protons and neutrons. The shape of the asymmetry term is [11]:

$$(E_{\rm S} = (A - 2Z)^2 / A) \dots (8)$$

It can be more easily understood by considering the fact that this term A goes to zero for A = 2Z and its effect is smaller for larger (A). Where N is the neutron number, Z is atomic number and A is the mass number.

4-Stopping power:

Many different names have been used for the quantity dE/dX names like energy loss, specific energy loss, differential energy loss, or stopping power. The stopping power dE/dX, defined as the energy lost by the incident particles per unit path length, total stopping power (S_t) is the sum of the electronic stopping power (S_e) , due to inelastic interaction with the target electrons, and the nuclear stopping power (S_n) induced by elastic collisions between the projectiles and the target nucleus[12].

$$S_t = S_e + S_n \qquad \dots \dots \dots \dots (9)$$

If the energy per atomic mass unit E/M of the incident particles is high, the nuclear contribution compared to the electronic one is negligible, that mean Nuclear stopping is only important at incident energies E < 100 keV, at higher energies nuclear stopping becomes negligible so $S_t = S_e$ [12,13].

4-1- Electron Stopping: The electronic stopping of α in elements S_e is derived from the stopping power of protons S_p for the same velocity by using[14]:

 Z_{α} is the alpha charge(α) and γ_{α} can be obtained from the simple polynomial fit.

With E represent alpha energy in keV/amu. C_i is coefficient. Note S_t can be converted to units of MeV/(mg/cm²) by multiplying by 0.6022/M².

4-2- Nuclear Stopping: The energy loss of the incident ion per unit Length S_n depends on the ion energy. The nuclear energy loss is small at very high energies, because fast particle have less interaction time with the scattering nucleus. Thus the nuclear energy loss tends to dominant towards the end of the range when ion has lost much of its energy, And The nuclear stopping S_n in eV/10¹⁵ atoms/cm2 for He-ions with incident energy E (in keV) is given by[15]:

Where M_1 , Z_1 refer to the ion and M_2 , Z_2 =substrate atom mass and atomic number. And the reduced ion energy ε , is defined as:

$$\varepsilon = \frac{32.53M_2E}{Z_1Z_2(M_1 + M_2)(Z_1^{0.23} + Z_2^{0.23})} \qquad \dots \dots \dots (13)$$

For $\varepsilon > 30$ keV, unscreened nuclear stopping is used, and $S_n(\varepsilon)$ simplifies to

$$S_n(\varepsilon) = \frac{ln\varepsilon}{2\varepsilon}$$
(14)

5- Neutron Yields:

The Yield of neutron (Y) detected per incident particle (alpha), for an ideal, thin, and uniform target and monoenergetic particles beam of incident energy E_b is given by [16].

Where n: is the number of target atoms per unit volume, t is the target thickness, σ is the reaction cross section, η is the alpha-detection efficiency. If the target is sufficiently thick, and there exist one atom per each molecule and taking the efficiency $\eta = 1$, then the resulting alpha yield is called the thick-target yield which is given by [17,18].

Where, N is the atomic number of target per unit volume, which is defined as follows:

Where, w is the abundant in the combination, ρ is the combination density, A is the mass number, N_A is the Avogadro's number, $\sigma_{(E)}$ is the cross section, dE/dX is the incident particle initial energy. For natural elements and if only one stable isotope is available in nature, then [19]

$$Yo = Y(E)$$
 ----- (18)

where (Yo) is the neutron yield per 10^6 bombarding particle for the natural element.

6- Results and Discussion:

The target (Calcium) has 24 isotopes, which are 34 Ca to 57 Ca. For this study (41 Ca - 50 Ca) that have four stable isotopes of observations (42 Ca, 43 Ca, 44 Ca and 46 Ca) table (1), in addition to isotope (48 Ca) with the long half-life that

for all practical purposes it can be considered stable as well as the rare ${}^{46}Ca$, are theoretically unstable on energetic grounds, but their decay has not been observed. Calcium also has a cosmogenic isotope, radioactive ${}^{41}Ca$, which has a half-life of 102,000 years. ${}^{41}Ca$ is produced by neutron activation of ${}^{40}Ca$. ${}^{41}Ca$ has received much attention in stellar studies because it decays to ${}^{41}K$, a critical indicator of solar-system anomalies. The most stable artificial radioisotope is ${}^{45}Ca$, with a half-life of 163 days [20]. The atomic mass Isotopes of elements (Ca and Ti) mentioned in this study have been taken [21] to calculate the binding energy are listed in table (1) as well as abundance[22], spin , parity[23] and half life[20].

isotopes	Atomic Mass(amu) [21]	B.E(MeV) P.W	Abundance % [22]	Half-life [20]	Spin & Parity [23]
⁴¹ Ca	40.96228	352.5606	-	1.02*10 ⁵ y	7/2-
⁴² Ca	41.95862	364.0414	0.647	Stable	0^+
⁴³ Ca	42.95877	371.9744	0.135	Stable	7/2-
⁴⁴ Ca	43.95548	383.1057	2.086	Stable	0+
⁴⁵ Ca	44.95619	390.5206	-	136 d	7/2-
⁴⁶ Ca	45.95369	400.9152	0.004	Stable	0^+
⁴⁷ Ca	46.95455	408.1917	-	4.536 d	7/2-
⁴⁸ Ca	47.95253	418.1371	0.187	6e+18 y	0^+
⁴⁹ Ca	48.95567	423.2837	-	8.718 m	3/2-
⁵⁰ Ca	49.95752	429.6367	-	13.9 s	0+
⁴⁴ Ti	43.95969	377.835	-	60.2y	0^+
⁴⁵ Ti	44.95813	387.3637	-	3.08056h	7/2-
⁴⁶ Ti	45.95263	400.5529	8.25	Stable	0^+
⁴⁷ Ti	46.95176	409.4333	7.44	Stable	5/2-
⁴⁸ Ti	47.94795	421.0601	73.72	Stable	0^+
⁴⁹ Ti	48.94787	429.2026	5.41	Stable	7/2-
⁵⁰ Ti	49.94479	440.142	5.18	Stable	0+
⁵¹ Ti	50.94661	446.5146	-	5.767m	3/2-
⁵² Ti	51.9469	454.323	_	1.67m	0^+
⁵³ Ti	52.94973	459.7584	-	32.7s	3/2-

Table (1): The atomic mass of isotopes used in the present work and another data.

We explain same properties of Ca(p,n)Ti reactions from calculated banding energy (BE), Q-value (Q), reduced mass (μ), threshold energy (E_{thr}) and separation energies of neutron (n), and we lasted in Table (2), from this tables we found that same of this reactions are excergic and the others are endoergic, in addition to other characteristics.

Reaction Type	Q – value (MeV) P.W	threshold energy (MeV) P.W	reduced mass (amu) P.W	separation energies (MeV) P.W
⁴¹ Ca(a,n) ⁴⁴ Ti	377.835	3.55327	3.646306	8.362935
⁴² Ca(a,n) ⁴⁵ Ti	387.3637	5.684025	3.654029	11.48078
⁴³ Ca(a,n) ⁴⁶ Ti	400.5529	0.073388	3.661453	7.933008
⁴⁴ Ca(a,n) ⁴⁷ Ti	409.4333	2.382606	3.668543	11.13131
⁴⁵ Ca(a,n) ⁴⁸ Ti	421.0601	2.208718	3.675371	7.414908
⁴⁶ Ca(a,n) ⁴⁹ Ti	429.2026	0.243427	3.681905	10.39459
⁴⁷ Ca(a,n) ⁵⁰ Ti	440.142	3.732079	3.688204	7.276487
⁴⁸ Ca(a,n) ⁵¹ Ti	446.5146	0.14511	3.694243	9.945467
⁴⁹ Ca(a,n) ⁵² Ti	454.323	2.734626	3.700084	5.146565
⁵⁰ Ca(a,n) ⁵³ Ti	459.7584	1.739391	3.705701	6.353007

Table (2): Calculated results for Ca(α,n)Ti reactions

The cross-section of $Ca(\alpha,n)Ti$ reactions for isotopes (⁴⁴Ti - ⁵³Ti) available in the literatures Labs (TENDL-2012)[24] has been taken into consideration and re-plotted, interpolated and analyzed by using the MATLAB computer program to obtain the cross-section for energy range (10 - 50) MeV in fine steps of (0.5MeV) as shown in figure (1).





We note from this figure that the best area of stability for the probability interaction involving all the curves start at energy approximately 15MeV (solid line) to 50MeV, an area that we have adopted for the calculations to get best results. After that, and depending on the energies of the incident Alpha and the targets of calcium isotopes (A=41-50) and using the program (SRIM 2013) [25] was calculated stopping power at these energies . It is the ability of the stopping power with cross-sections at corresponding energies we calculated the neutron yields ($n/10^6$ d) theoretically, shown in figure (2).



Figure (2): The neutron yield of Ca(α ,n)Ti reaction at energy rang (10-50)MeV for Ca mass number (41-50)

We know increasing the mass number with proven atomic number for calcium isotopes that meaning an increase in the number of neutrons and the result will directly affect in the asymmetry energy, which was calculated for calcium isotopes, which we used to extract the empirical formula between the mass number and neutron yield shown in figure (3), for the incident Alpha energies (10-15) MeV in fine steps of (5 MeV).



Asymmetry

Fig (3). The neutron yield with asymmetry of Ca target isotopes for different Alpha energy induced reactions at (10 - 50) MeV

And the formula that was extracted by fitted for all these curves:

$$Y = \alpha \beta \ ^{Es} E s^{\gamma} \quad \dots \dots \quad (19)$$

Where Y represent neutron yield. Es represent asymmetry energy. α , β and γ represents the first coefficients by different values for each energy as shown in Table (3).

Table (3) :Primary coefficients at different incident alpha energies when fitted curve between yield and asymmetry to get find coefficients

Alpha energy(MeV)	А	β	Г	
10	5.847246	1.02E-01	1.13795	
15	7.72E+01	6.27E-02	9.83E-01	
20	9.68E+01	6.11E-02	8.48E-01	
25	1.01E+02	6.40E-02	8.24E-01	
30	1.02E+02	6.71E-02	8.13E-01	
35	1.02E+02	6.93E-02	8.05E-01	
40	1.02E+02	7.08E-02	7.99E-01	
45	1.02E+02	7.19E-02	7.95E-01	
50	1.02E+02	7.27E-02	7.92E-01	

From this table we draw the relationship between energy and the different values for each coefficient, the fitted expressions for each coefficient give us following formulas:

$$\begin{aligned} \alpha &= B1 \, e^{(B2 \, E)} + B3 \, e^{(B4 \, E)} & \dots \dots \dots (20) \\ \beta &= B5 \, E^{B6} + B7 \, e^{(B8 \, E)} & \dots \dots \dots (21) \\ \gamma &= B9 \, (E - B10)^{B11} & \dots \dots \dots (22) \end{aligned}$$

And gives the following values of parameters: [B1 = -2443.5, B2 = -0.30519, B3 = 102.46, $B4=0.97403*10^{-04}$, B5 = 0.9665, B6 = -0.5926, B7 = -0.27937, B8 = -0.05020, B9 = 0.8961345, B10 = 1.49268, B11 = -0.03539].

We have obtained formula of a set of $Ca(\alpha,n)Ti$ reactions has been used to calculate the neutron yields for each Ca isotopes at energy rang between (15 - 50) MeV and compared with the adopted neutron yields calculated from the fitting expressions and shown to be in a good agreement, the comparison of result shown in table (4)

Table (4). The comparison between the	value of neutron yi	rield from the	coretically and	present work	(empirical
formula)					

Energy = 15 MeV				Energy = 20 MeV			
Mass number	Yield Theory	Yield P.W	Error %	Mass number	Yield theory	Yield P.W	Error %
41	2.18867	1.875161	14.32418	41	3.20474	3.907576	21.93112
42	5.42244	5.875613	8.357366	42	10.64807	10.14735	4.70242
43	9.82835	9.291508	5.462174	43	14.23652	14.37318	0.959958
44	10.21789	10.42822	2.058432	44	15.34688	14.91081	2.841392
45	8.62891	9.294011	7.707824	45	10.80398	12.49172	15.62149
46	8.0914	6.93943	14.23696	46	10.38187	8.859522	14.66352
47	3.86349	4.476616	15.86974	47	4.80287	5.466787	13.82334
48	2.99153	2.547835	14.83169	48	3.66805	2.991006	18.45788
49	0.74096	1.297684	75.13545	49	0.94081	1.469829	56.23022
50	0.40149	0.598549	49.08188	50	0.56736	0.655953	15.61499
Energy = 25 MeV					Energy = 3	0 MeV	
Mass number	Yield Theory	Yield P.W	Error %	Mass number	Yield theory	Yield P.W	Error %
41	3.53422	4.401344	24.53508	41	3.71933	4.641864	24.80378
42	11.98828	11.14888	7.001821	42	12.45565	11.60991	6.790001
43	15.52517	15.61059	0.550194	43	16.09663	16.19124	0.587763
44	16.7124	16.11056	3.601168	44	17.26257	16.71971	3.144735
45	11.664	13.48164	15.58331	45	12.15842	14.04487	15.51561
46	11.2959	9.579684	15.19326	46	11.76259	10.04365	14.61359
47	5.38913	5.936669	10.16007	47	5.78998	6.277498	8.420034
48	3.97639	3.268718	17.79685	48	4.1632	3.492541	16.10921
49	1.08544	1.619353	49.18864	49	1.18837	1.751301	47.37001
50	0.69718	0.729686	4.662535	50	0.78872	0.799968	1.426141
	Energy = 3	5 MeV		Energy = 40 MeV			
Mass number	Yield Theory	Yield P.W	Error %	Mass number	Yield theory	Yield P.W	Error %
41	3.85423	4.797047	24.46186	41	3.94866	4.913645	24.4383
42	12.75922	11.89569	6.767874	42	12.96944	12.10191	6.689002
43	16.46886	16.55235	0.506971	43	16.72051	16.80365	0.497228
44	17.6065	17.11241	2.806309	44	17.83939	17.37873	2.582251
45	12.49658	14.42662	15.44457	45	12.72349	14.6824	15.39598
46	12.0592	10.37419	13.97283	46	12.25577	10.59536	13.54796
47	6.07058	6.531188	7.587541	47	6.25962	6.701858	7.064936
48	4.29358	3.665456	14.62937	48	4.38087	3.782847	13.65079
49	1.26043	1.856542	47.29437	49	1.30789	1.928789	47.4733

50	0.85331	0.857622	0.505349	50	0.89588	0.897691	0.202153	
Energy = 45 MeV				Energy = 50 MeV				
Mass number	Yield Theory	Yield P.W	Error %	Mass number	Yield theory	Yield P.W	Error %	
41	4.01701	5.007862	24.6664	41	4.06912	5.08692	25.01279	
42	13.1233	12.26031	6.57599	42	13.24044	12.38518	6.459445	
43	16.90252	16.98211	0.470853	43	17.03839	17.10627	0.398389	
44	18.00729	17.55157	2.530756	44	18.13329	17.65094	2.660052	
45	12.88477	14.83611	15.14458	45	13.00449	14.90661	14.62666	
46	12.39539	10.72159	13.50343	46	12.49965	10.76838	13.85052	
47	6.39549	6.796473	6.269779	47	6.49844	6.826232	5.044161	
48	4.44348	3.847073	13.42207	48	4.49111	3.865223	13.93613	
49	1.34276	1.968185	46.57755	49	1.37101	1.97868	44.32277	
50	0.92646	0.919597	0.740821	50	0.94905	0.925284	2.504209	

The comparison shows that the calculated results are in agreement to the behavior of the theoretical curve range, there is a simple systematic deviation as shown in Figure (4) for all Ca isotopes at different energy.





Figure (4): The comparison between neutron yields calculated from the theoretically relationship and fitting expressions for Ca(a,n)Ti

The reason of the deviation is the large interval of long energy rang. It is noted that the neutron yield for energies between (10-14) was not included with the rest of the table because of the big difference between the theoretical values and the calculated values from empirical formula, this reason was determined the area of energy in the figure (1) at the beginning of the work.

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