

Statistical model analysis of cross sections of (n,t) and $(n,{}^3\text{He})$ reactions induced by 14.6 MeV neutrons on target nuclei with $A = 27$ to 59

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Total cross sections of 14.6 MeV neutron induced reactions (n,n') , (n,p) , (n,d) , (n,α) , (n,t) , and $(n,{}^3\text{He})$, on the target nuclei in the mass region $A = 27$ to 59, have been calculated (for the first stage decay) by the Hauser-Feshbach method using a unified set of optical model parameters. The strong reaction channels are described well by the calculations. The (n,t) reaction on target nuclei in the $(2s,1d)$ shell seems to proceed predominantly via statistical processes; for heavier nuclei nonstatistical contributions become important. In the case of $(n,{}^3\text{He})$ reactions, the few experimentally measured cross sections are much higher than those obtained by theoretical calculations.

[NUCLEAR REACTIONS (n,x) cross sections at 14.6 MeV; Hauser-Feshbach analysis.]

I. INTRODUCTION

In the interactions of 14 MeV neutrons with nuclei, radiative neutron capture has relatively low probability. On the other hand, reactions such as (n,n') , (n,p) , (n,d) , and (n,α) as well as processes involving the emission of two nucleons, such as $(n,n'p)$ and $(n,n'\alpha)$ in the lighter mass region and $(n,2n)$ in the heavier mass region constitute relatively strong reaction channels. Reactions such as (n,t) and $(n,{}^3\text{He})$ are also energetically possible but in the medium and heavy mass regions are rather rare.

Fast neutron radiative capture is a special case and can be well treated by the direct-semidirect theory (cf. Refs. 1–3). As far as (n,n') , (n,p) , (n,α) , and $(n,2n)$ reactions are concerned, extensive statistical model calculations, in several cases using the Hauser-Feshbach method,⁴ have been carried out (cf. Refs. 5–18), and in the medium mass region the agreement between experimental data and theoretical calculations is generally good. Precompound effects^{11–18} have also been included in some calculations. In recent years such calculations have achieved considerable sophistication (cf. Ref. 18) and the available codes can provide with reasonable accuracy the desired cross section data on those reactions, especially with regard to fusion reaction technology (FRT). The $(n,n'p)$ and $(n,n'\alpha)$ reaction cross sections have been estimated by two-step Hauser-Feshbach calculations (cf. Ref. 19), though as yet it is difficult to comment whether the calculation would reproduce the excitation function successfully, since the available experimental data base at

energies other than 14 MeV is rather meager.²⁰

The (n,t) cross section for very light nuclei is exceptionally large due to deuteron and triton cluster formation which facilitates direct reactions such as deuteron “pickup” and triton “knock-out.” The occurrence of such direct processes has been demonstrated by analysis of the emitted triton spectra (cf., e.g., Refs. 21–23). For (n,t) and $(n,{}^3\text{He})$ reactions in the medium and heavy mass regions, however, no information regarding their mechanisms is available. The reaction (n,t) in which, as in $({}^3\text{He},p)$, both $\Delta T = 0$ and $\Delta T = 1$ are possible, is more complicated and in general more difficult to interpret²⁴ than, e.g., the (p,t) and $(n,{}^3\text{He})$ two-nucleon transfer reactions, for which only $\Delta T = 1$ is possible. The cross sections for the (n,t) and $(n,{}^3\text{He})$ reactions are very low and can be currently measured only by the activation technique. In both those reactions most of the transitions lead to low-lying discrete levels of the residual nucleus.

In the literature, although some older reports^{25–27} on estimating cross sections of some isolated (n,t) and $(n,{}^3\text{He})$ reactions using the simple evaporation theory exist, any systematic and detailed analysis was not attempted. This was partly due to the fact that for such rare reactions even no good activation cross section data existed. In recent years, systematic experimental studies in the medium and heavy mass regions on 14.6 MeV neutron induced (n,t) reactions have been carried out at Jülich^{28–30} and Debrecen^{31,32} and on $(n,{}^3\text{He})$ reactions at Jülich.^{33,34} Those studies have provided now some accurate cross section data to make theoretical analysis worthwhile. In an at-

tempt to analyze their (n, t) data, Sudar and Csikai³² recently attempted a Hauser-Feshbach analysis for the target nuclei ^{27}Al , ^{32}S , ^{55}Mn , ^{59}Co , and ^{58}Ni . We have performed complete Hauser-Feshbach calculations on the (n, t) and $(n, ^3\text{He})$ reactions on the target nuclei in the mass

region $A = 27$ to 59 using a unified set of optical model parameters and without introducing any normalization factors. Preliminary results were already described³⁵; now we give a detailed report on our calculations.

II. CALCULATIONS

The Hauser-Feshbach expression^{36, 37} of the total cross section for the excitation of a state at excitation energy E_B^* and with spin I_B , via the reaction $A(a, b)B$, reads

$$\sigma(E_B^*, I_B) = \sum_J^{\max} \sigma_{\text{form}}(J) G(E_B^*, I_B, J) / g(J). \quad (1)$$

In Eq. (1), $\sigma_{\text{form}}(J)$ describes the cross section for the formation of a compound nucleus with spin J :

$$\sigma_{\text{form}}(J) = \pi \lambda_1^2 \frac{2J+1}{(2I_A+1)(2I_a+1)} \sum_{s_1=|I_A-I_a|}^{I_A+I_a} \sum_{l_1=|J-s_1|}^{J+s_1} T_{l_1}(E_a). \quad (2)$$

The partial width for the decay of a compound nucleus state with spin J to a state of the residual nucleus at an excitation energy E_B^* and with spin I_B reads

$$G(E_B^*, I_B, J) = \sum_{s_2=|I_B-I_b|}^{I_B+I_b} \sum_{l_2=|s_2-J|}^{s_2+J} T_{l_2}(E_B^*). \quad (3)$$

The total width $g(J)$ for the decay of the compound nucleus into all open channels (denoted by primes) $b' + B'$ is split into two parts,

$$g(J) = \sum_{b'} \sum_{l_2'} \sum_{s_2'=|l_2'-J|}^{l_2'+J} \sum_{I_B=|s_2'-I_b|}^{s_2'+I_b} \left[\sum_{E_B^*=0}^{E_c} T_{l_2'} + \int_{E_B^*=E_c}^{E_B^*, \max} T_{l_2'} \rho(E_B^*, I_B) dE_B^* \right], \quad (4)$$

thus replacing the summation over transmission coefficients T_l of discrete levels by an integration over level densities $\rho(E^*, I)$ at the beginning E_c of the "continuum region."

The program calculates transmission coefficients T_l via an optical model without spin-orbit coupling. All $T_l > 10^{-3}$ were taken into account. In the summation over J in Eq. (1) no limiting critical angular momentum J_{\max} —as necessary in heavy ion reactions^{38, 39}—is used. For each reaction product all the low-lying levels^{40, 41} extending up to an excitation energy beyond which the level density could be treated statistically were considered. In general, this covered an excitation energy region up to about 3 MeV.

The energy levels in the continuum were obtained using the composite level density formula as given by Gilbert and Cameron⁴² in the following form (see also Ref. 43):

$$\rho(E^*, I) = \omega(E^*) F(E^*, I). \quad (5)$$

In this expression the spin dependence is contained in the second factor

$$F(E^*, I) = \frac{2I+1}{2\sigma^2} \exp[-(I + \frac{1}{2})^2 / 2\sigma^2],$$

while the first factor $\omega(E^*)$ contains the energy dependence [apart from the slight energy dependence of the spin-cutoff parameter σ in $F(E^*, I)$]:

$$\omega_{1,2}(E^*) = \begin{cases} \frac{1}{T} \exp[(E^* - E_0)/T], \\ \exp(2\sqrt{aU}) / 12\sqrt{2} a^{1/4} U^{5/4} \sigma. \end{cases}$$

The "constant temperature" approximation ω_1 is used for low excitation energies $E^* \leq E_x$, while the Fermi gas expression is applied for $E^* > E_x$. The energy U denotes the excitation energy E^* minus the pairing energy Δ . The values of E_x, E_0 , the nuclear temperature T at the excitation energy $E^* = E_x$, as well as the pairing energy were obtained from Ref. 42. The level density parameter a was either taken from Ref. 42 or, in cases where no value was available, the approximation $a \sim A/7.5$ was employed. The spin-cutoff parameter σ was obtained from the formula given in Ref. 42 but using the corrected numerical factor of Ref. 44:

$$\sigma^2 = 0.1459 \sqrt{aU} A^{2/3}. \quad (6)$$

The Q values of the reactions were taken from the

TABLE I. Optical model parameters used for calculation of transmission coefficients.

Particle	Potential (MeV)	Real		Potential and type (MeV)	Imaginary		Ref.
		Radius (fm)	Diffusivity (fm)		Radius (fm)	Diffusivity (fm)	
n	$56.3-0.32E-24(N-Z)/A$	$1.17A^{1/3}$	0.75	$13.0-0.25E-12(N-Z)/A^a$ SW-DERIV	$1.26A^{1/3}$	0.58	46
p	$54.0-0.32E+24(N-Z)/A+0.4Z/A^{1/3}$	$1.17A^{1/3}$	0.75	$11.8-0.25E+12(N-Z)/A^a$ SW-DERIV	$1.32A^{1/3}$	$0.51+$ $0.7(N-Z)/A$	46
d	$81.0-0.22E+2Z/A^{1/3}$	$1.15A^{1/3}$	0.81	$14.4+0.24E$ SW-DERIV	$1.34A^{1/3}$	0.68	47
t	152.0	$1.24A^{1/3}$	0.67	25.4 SW	$1.44A^{1/3}$	0.82	48
^3He	158.1	$1.24A^{1/3}$	0.56	24.5 SW	$1.35A^{1/3}$	1.07	49
α	183.7	$1.40A^{1/3}$	0.56	26.6 SW	$1.40A^{1/3}$	0.56	50

^a In case of negative values, a figure of zero is used. All E values are in MeV and refer to c.m. system.

mass tables of Wapstra and Gove.⁴⁵

The used optical model parameters for neutrons and protons were taken from the work of Becchetti and Greenlees,⁴⁶ for deuterons from Perey and Perey,⁴⁷ for tritons from Ragaini *et al.*,⁴⁸ for ^3He from Luetzelschwab and Hafele,⁴⁹ and for α particles from Bock *et al.*⁵⁰ The data for tritons and ^3He particles, which are emitted with low energies, are not known with the same accuracy as for the other lighter particles. The selected optical model parameters for tritons and ^3He particles are listed in Table I together with the parameters for other particles.

The computation of Eq. (1) was carried out on an IBM 370/168 computer using the program HELGA (cf. Ref. 43), originally written by Penny.⁵¹ It

allows inclusion of up to ten binary scattering and reaction channels $A(a, b)B$. Cross sections were calculated for the discrete levels fed and for the levels in the continuum in energy intervals of 0.1 MeV up to the maximum excitation energy of the final nucleus. In the calculation of the production cross sections, emission of further nucleons from the produced nucleus was not considered. This should not cause any errors in the calculated (n, t) and $(n, ^3\text{He})$ production cross sections because of the highly negative Q values for these reactions. Calculations by the program CASCADE (written by Pühlhofer⁵²) show that the (n, α) production cross section is also not too much affected; however, as a result of further nucleon and α emission the real production cross

TABLE II. Cross sections of some strong reaction channels induced by 14.6 MeV neutrons.

Target nuclide	$\sigma(n, n'x)$ mb		$\sigma(n, px)$ mb		$\sigma(n, \alpha x)$ mb	
	theor.	theor.	theor.	exp. ^a	theor.	exp. ^a
Al-27	676	166		75 ± 4	248	121 ± 6
Si-28	390	588		226 ± 30	166	$[250 \pm 50]^b$
P-31	766	180		97 ± 15	224	118 ± 15
S-32	440	430		254 ± 25	316	$[300 \pm 60]^b$
K-39	747	221		354 ± 54	324	$[200 \pm 40]^b$
K-41	1222	60		51 ± 8	38	39 ± 8
Ca-40	904	268		$[350 \pm 70]^c$	162	138 ± 20
Sc-45	1277	88		57 ± 6	9	56 ± 6
Ti-46	1137	200		166 ± 15	66	$[100 \pm 20]^b$
Cr-50	915	524		$[277 \pm 21]^d$	30	$[121 \pm 8]^d$
Fe-54	916	529		332 ± 30	73	100 ± 10
Co-59	1510	23		73 ± 10	15	30 ± 2

^a All the experimental values have been taken from the compilation of Qaim (Ref. 57) unless otherwise stated; they refer to the activation cross sections of the (n, p) and (n, α) reactions, i.e., without any contributions from $(n, n'p)$ and (n, pn) , or $(n, n'\alpha)$ and $(n, \alpha n)$ reactions.

^b From systematics of (n, α) reaction cross sections (Ref. 55).

^c From systematics of (n, p) reaction cross sections (Ref. 56).

^d From the compilation of Paulsen (Ref. 54).

sections might be lower than the calculated values given in Table II by up to ~50% for (n, n') and by ~30% for (n, p) reactions.

III. RESULTS AND DISCUSSION

Cross sections were calculated for (n, n') , (n, p) , (n, d) , (n, α) , (n, t) , and $(n, {}^3\text{He})$ reactions on target nuclei in the mass region $A = 27$ to 59. Calculations were performed for incident neutron energies of 14.0, 14.2, 14.4, 14.6, 14.8, and 15.0 MeV. The calculated cross sections for the main reaction channels (n, n') , (n, p) , and (n, α) showed little dependence on small variations in the incident neutron energy. This observation is in agreement with the experimental results. Since the maxima of the excitation functions of those reactions occur around 14 MeV, in the energy region 14 to 15 MeV their reaction cross sections are relatively independent of the incident neutron energy. The cross section for the relatively weaker (n, d) reaction channel showed some increase over the energy range of 14 to 15 MeV; those data will be discussed in detail elsewhere. In the case of the weak reaction channels (n, t) and $(n, {}^3\text{He})$, on the other hand, due to the highly negative Q values a strong dependence of the cross section on small changes in the incident neutron energy was observed. We limit ourselves to a discussion of the results of theoretical calculations at 14.6 MeV since most of the experimental information has been reported for this neutron energy.

The calculated cross sections for (n, n') , (n, p) , and (n, α) reactions are given in Table II. For those reactions the major part of the cross section is constituted by transitions to the continuum. The (n, n') cross sections obtained by the present theoretical calculations are of the order of those expected from the systematics (cf. Refs. 6 and 53). In the case of (n, p) and (n, α) reactions, a more stringent test is possible since many of the reaction cross sections have either been measured experimentally or can be deduced accurately from the systematics. A comparison of the results of theoretical calculations with the experimental data⁵⁴⁻⁵⁷ for those two reactions is given in Table II. With a few exceptions, our calculated data are in agreement with the experimental data within a factor of 2. This can be considered as rather good since the experimental value gives the summed cross section to final states below the particle threshold while the calculated value corresponds to the total cross section, and in view of the fact that in the present calculations unified set of optical model and level density parameters have been used. This observation adds confidence to our calculations on the weaker reaction channels

TABLE III. Cross sections of some weak reaction channels induced by 14.6 MeV neutrons.

Target nuclide	$\sigma(n, t)$ μb		$\sigma(n, {}^3\text{He})$ μb	
	theor.	exp. or from [systematics] ^a	theor.	exp. ^b
Al-27	2860	3000 \pm 400 ^c	<0.01	
Si-28	energetically not possible		0.7	
P-31	1400	[800 \pm 300]	<0.01	\leq 13
S-32	9	7.2 \pm 1.6	560	
K-39	500	184 \pm 37 ^c	113	
K-41	380	[150 \pm 60]	<0.01	6 \pm 3
Ca-40	6	27 \pm 8	200	
Sc-45	90	[70 \pm 20] [800 \pm 200] ^c	0.02	9 \pm 4
Ti-46	<0.1	115 \pm 35	2.0	
Cr-50	<0.1	66 \pm 20	7.4	
Fe-54	<0.1	105 \pm 35	15.1	
Co-59	70	640 \pm 130 ^c	<0.01	4.6 \pm 2.1

^a All values taken from the works of Qaim and Stöcklin (Refs. 29 and 30) unless otherwise stated.

^b Values from Qaim (Refs. 33 and 34).

^c Values from Csikai *et al.* (Refs. 31 and 32).

described below.

The calculated cross sections for (n, t) reactions are given in Table III and are compared with those obtained experimentally or from the systematics. For (n, t) reactions on target nuclei in the mass region $A = 27$ to 40 the theoretical calculations and experimental cross sections agree within a factor of 2 to 3. A similar conclusion was reached by Sudar and Csikai³² in the case of ${}^{27}\text{Al}$ and ${}^{32}\text{S}$. For nuclei with mass number above 40 our calculated (n, t) cross sections are significantly lower than the experimental values. Sudar and Csikai,³² on the other hand, found good agreement between experimental and theoretical (n, t) cross sections for ${}^{55}\text{Mn}$, ${}^{59}\text{Co}$, and ${}^{58}\text{Ni}$ as well. It should, however, be mentioned that Sudar and Csikai³² used level density parameters in the neutron channel which they determined from a fit of the calculated (n, α) excitation function to the experimental data. Since small variations in a in the neutron channel influence all the reaction cross sections appreciably, we did not do such a data fitting. Our calculations suggest that the emission of tritons from nuclei in the $(2s, 1d)$ -shell proceeds predominantly via statistical processes. In heavier nuclei some nonstatistical processes may also be involved. Such behavior is in agreement with that found in (t, p) reactions on Ni isotopes.⁵⁸

The data for the $(n, {}^3\text{He})$ reactions are also given in Table III. The few experimental cross section values existing over the mass range of $A = 27$ to 59 are much higher than those obtained

by theoretical calculations. Further experimental data are needed to describe the mechanism of ($n, {}^3\text{He}$) reactions.

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