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Thermonuclear reaction rates from (p, n) reactions

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Abstract. Thermonuclear reaction rates for the temperature range $1 \leq T_9 \leq 5$ have been extracted from experimentally measured (p, n) cross sections for ^{45}Sc ^{50}Ti, ^{51}V, ^{54}Cr, ^{55}Mn and ^{59}Co nuclides below 5 MeV bombarding energy. These reaction rates are important in the build-up of medium and heavy nuclides in the stellar evolution process and nucleosynthesis. To enhance the usefulness of these reaction rates in astrophysical calculations, they have been fitted to an analytic function of temperature, valid throughout the temperature range considered here.

Keywords. (p, n) reaction; ^{45}Sc, ^{50}Ti, ^{51}V, ^{54}Cr, ^{55}Mn, ^{59}Co targets; thermonuclear reaction rates.

1. Introduction

Astrophysical studies involving the synthesis of heavier elements duiing the carbon, oxygen and silicon burning stages of stellar evolution require a large number of thermonuclear reaction rates in the temperature range 10^9 °K to 10^{10} ° K. This process of building up of heavier nuclides is known as 'nucleosynthesis'. Mathematically, the process is represented by a set of coupled differential equations, the coefficients of which are proportional to the nuclear reaction rates (Vlieks *et al* 1974). It is clear that an enormous number of nuclear reaction rates are required for such studies. For example, a typical calculation of thermonuclear burning of carbon and oxygen fuels leading to nuclides in the vicinity of mass $A = 56$ involves more than 500 individual nuclear reactions, each of which must be known as a function of temperature (Truran 1972). These reaction rates are obtained either from calculations using experimentally determined cross sections or in cases where cross sections have not or cannot be measured from relevant theories. In order to establish the validity and prediction accuracies of such theories, experimental measurement of cross sections for suitable nuclear reactions are also necessary. One such attempt has been made here to calculate the thermonuclear reaction rate (TNRR) as a function of temperature from the measured low energy (p, n) reaction cross sections on some medium weight nuclei. Fowler (1969) has suggested that much more research on the interaction of protons, alpha particles, neutrons with intermediate mass nuclei in the energy range 1 to 100 MeV is needed before convincing results can be obtained. This is particularly true in regard to current attempts to account for less abundant nuclides in the range $29 \leq A \leq 55$.

2. Thermonuclear reaction rate

The heart of the nucleosynthesis process in a stellar evolution is the thermonuclear reaction (Burbidge *et al* 1957, Clayton 1968, Vlieks *et al* 1974). The stellar reaction rate is the rate at which a specific nuclear reaction takes place in the stellar environment. The factors contributing to this rate are the cross section for the reaction and the temperature of the stellar environment which determines the energy distribution of the colliding particles. For reactions between the non-identical nuclear species, the reaction rate is defined as $RR = n_1 n_2 \langle \sigma v \rangle$ reactions/unit volume/sec., where n_1, n_2 are the number densities of the two species and $\langle \sigma v \rangle$ is the average of the energy dependent cross section over the relative velocity, v, distribution of the two species. If one makes the usual assumption of a Maxwell-Boltzmann velocity distribution for the nuclei at temperature T within a star, we can write (Vlieks *et al* 1974),

$$\langle \sigma v \rangle = \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} (kT)^{-3/2} \int_{|Q|}^{\infty} E\sigma(E)\, e^{-E/KT}\, dE \tag{1}$$

where k = Boltzmann constant, μ = reduced mass, E = centre of mass energy, $Q = Q$ value of the reaction if it is endoergic, zero otherwise, T = absolute temperature and $\sigma(E)$ = energy dependent cross section. At low energies, the main factors contributing to σ (in the case of interaction between two charged particles) are the coulomb penetrability factor which is proportional to $\exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar v}\right)$ (Z_1 and Z_2 are charge numbers of interacting particles) and the quantum mechanical geometrical factor which is proportional to $\lambda\!\!\!^{-2}$ ($\lambda\!\!\!^{-}$ is the de Broglie wavelength) or $1/E$. Based on these considerations one can define (Clayton 1968) the cross section at low energy as a product of three separate energy dependent factors:

$$\sigma(E) = S(E)\frac{1}{E}\exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar v}\right) \tag{2}$$

$S(E)$ represents the intrinsic nuclear part of the probability for the occurrence of a nuclear reaction which may not be very sensitive to energy variation whereas the other two terms, as pointed out earlier, are of non-nuclear nature and are strongly dependent on energy. In general, $S(E)$ may be a slowly varying function of E. Substituting for $\sigma(E)$ from (2) in (1), we get

$$\langle \sigma v \rangle \propto \int_{|Q|}^{\infty} S(E) \exp(-bE^{-1/2}) \exp\left(-\frac{E}{kT}\right) dE \tag{3}$$

where $b = 31\cdot28\ Z_1 Z_2 A^{1/2}$, $A = A_1 A_2/(A_1 + A_2)$ and A_1 and A_2 are the mass numbers of the interacting particles. As this expression tends to zero, for large E through the factor $\exp(-E/kT)$ and for small E through the factor $\exp(-bE^{-1/2})$, the major contribution to the integral will come from values of the energy that are such that the exponential factor is near its maximum. The probability of reactions occurring is thus significant over a narrow energy region, so narrow that $S(E)$

may be assumed to remain constant over this narrow band of energies. A good approximation to this narrow energy region is a Gaussian-shaped curve centred at energy (Vlieks 1974)

$$E_0 = 0\cdot 122\,(Z_1 Z_2 A\,(T_9)^2)^{1/3}\ \text{MeV} \tag{4}$$

with a full width at half maximum of

$$\triangle E = 0\cdot 237\,(Z_1^2\, Z_2^2\, A\,(T_9)^5)^{1/6}\ \text{MeV} \tag{5}$$

(T_9 is temperature expressed in units of 10^9 °K). A more usual form of quoting the stellar reaction rates is given by

$$RR = N_A \langle \sigma v \rangle \tag{6}$$

where N_A = Avogadro number. This expression is independent of the number densities of the interacting particles.

3. Reaction rates from nuclear cross section

3.1 *Experimental measurements*

The total (p, n) reaction cross sections on ^{45}Sc, ^{50}Ti, ^{51}V, ^{54}Cr, ^{55}Mn and ^{59}Co (Iyengar *et al* 1967, Sekharan *et al* 1966, Kailas *et al* 1974, 1975 *a*) measured earlier at the Van de Graaff laboratory at Trombay have been used in this analysis to extract the TNRRs of interest in the field of astrophysics. The experimental measurements were carried out utilising a 4π geometry neutron counter (Sekharan 1965). The targets were prepared by evaporating the proper materials either in elemental form or in the oxide form on to thick Ta backings. The target thickness in all the cases was $\sim$5 keV for 3 MeV protons. The details of experimental measurements are published elsewhere (Kailas *et al* 1975 *a*). The overall error in the (p, n) reaction cross section measurements is between $\pm$ 15 to $\pm$ 20%. In all cases the fine structure (p, n) excitation functions measured in small energy steps ($\sim$ 5 keV) were averaged over large energy intervals (200 to 500 keV) to smooth out the excitation functions. These averaged excitation functions were used for the subsequent analysis in the present work.

3.2 *Theoretical RR*

At low energies, the charged particle reactions on medium weight nuclei generally proceeded through a compound nucleus with closely spaced states with narrow widths. Utilising the fact that these overlapping compound nuclear states contribute to the cross section, one can define an effective averaged cross section for this process (Truran 1972) as (for p, n reaction)

$$\sigma_{p,n} = \sum_J \pi^2 \lambda_p^2 \frac{\Gamma_p \Gamma_n}{D\,(U, J)\,\Gamma} \frac{(2J+1)}{(2I+1)} \tag{7}$$

where J = compound nuclear spin, I = spin of the target nucleus, $D\,(U,J)$ = average level spacing of levels with spin J at excitation energy U, Γ_p, Γ_n and Γ are the proton, neutron and total widths. Thus the theoretical calculation of σ reduces to the estimation of the partial widths and level density. From the relation $T = 2\pi(\Gamma/D)$ where T is the transmission coefficient obtainable from optical model calculations, one can evaluate Γ/D and hence determine σ. This in turn leads to the evaluation of RR. The above expression for cross section gets simplified, if $\Gamma_n \gg \Gamma_p$, to the form

$$\sigma_{p,n} \approx \pi \lambda\!\!\!^{-}{}_p^2 \sum_l (2l+1)\, T_l \approx \sigma_{\mathrm{abs}} \tag{8}$$

σ_{abs} is the absorption cross section. Thus the theoretical attempt to calculate TNRR rests chiefly in finding realistic and consistent optical potentials. Kailas *et al* (1975 *b*) have determined a set of proton optical model potentials at sub-Coulomb energies for the nuclides considered here. But no attempt has been made here to use them to get theoretical RR as the optical potentials are not unique and there may be large uncertainties and deviations if TNRRs are calculated theoretically using a common set of optical model parameters. However, these theoretical calculations are useful to get an order of magnitude of the reaction rate.

3.3 *Extraction of RR from experimental measurements*

As regards the experimental evaluation of TNRR, it is clear that to get the reaction rates of interest one must integrate $\sigma(E)$ $(\sigma_{p,n})$ with the distribution $E \exp(-E/kT)$. One could simply integrate numerically the values of $\sigma(E)$ measured at experimentally convenient energy intervals. To improve integration it is better to fit the averaged (p, n) excitation function by a smooth curve and integrate the fitted curve in smaller energy increments. Following the procedure of Vlieks *et al* (1974), the averaged (p, n) excitation functions were fitted to an empirical function as given below:

$$\sigma_{p,n}(E) = \frac{1}{E} \sum_{i=1}^{5} a_i \exp\left(-\frac{b}{\sqrt{E}}\right) E^{i-1} \tag{9}$$

a_i's and b are the parameters determined by least squares procedure as described in the above work of Vlieks *et al* (1974).

The theoretical fittings obtained for the (p, n) cross sections by this procedure are shown in figures 1–6. In figure 5, we have along with σ, plotted $S(E)$, the specific nuclear contribution to σ as a function of energy. It is clear from the figure $S(E)$ is slowly varying function of energy. Once the parameters a_i's and b required for $\sigma(E)$ were determined, eq. (1) was numerically integrated using standard Simpson's rule technique, from $|Q|$, the absolute Q value of the (p, n) reaction to about 5 MeV, approximately the highest energy measured. This procedure is justified, at least for temperatures in the range $T_9 = 1$ to 5 as the contribution to TNRR from above 5 MeV would be quite negligible (at the most 10% for $T_9 = 5$). A typical plot of the integrant of the RR expression given in eq. (1), for $T_9 = 2$, 3 for ^{55}Mn (p, n) ^{55}Fe reaction which has been shown in figure 7 justifies the above statements. The thermonuclear reaction rates calculated at temperatures between $T_9 = 1$ to 5 along with E_0 and E values for the reactions studied are tabulated in table 1. These TNRR values are expected

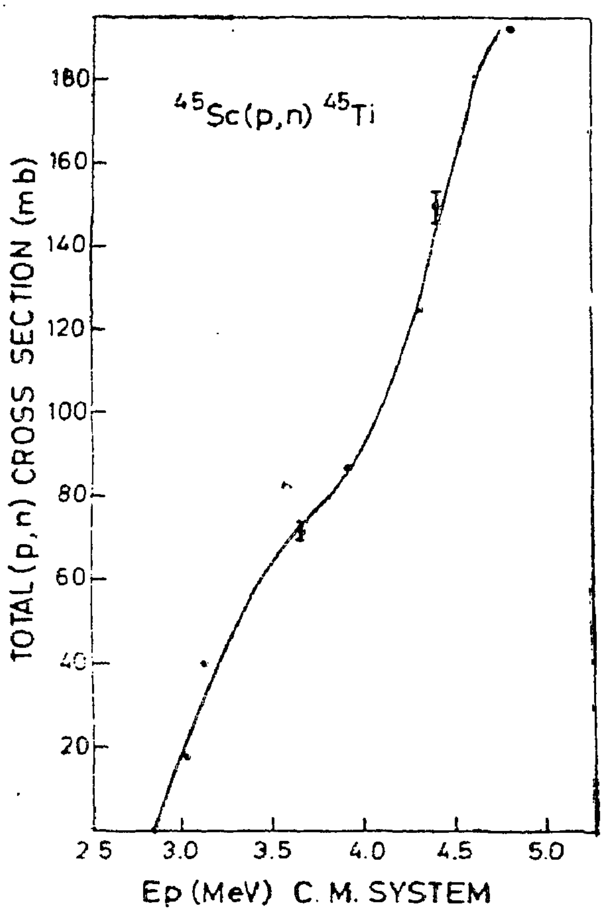

Figure 1. Averaged (p, n) excitation function for $^{45}Sc(p,n)^{45}Ti$ reaction and the polynomial fit to the same.

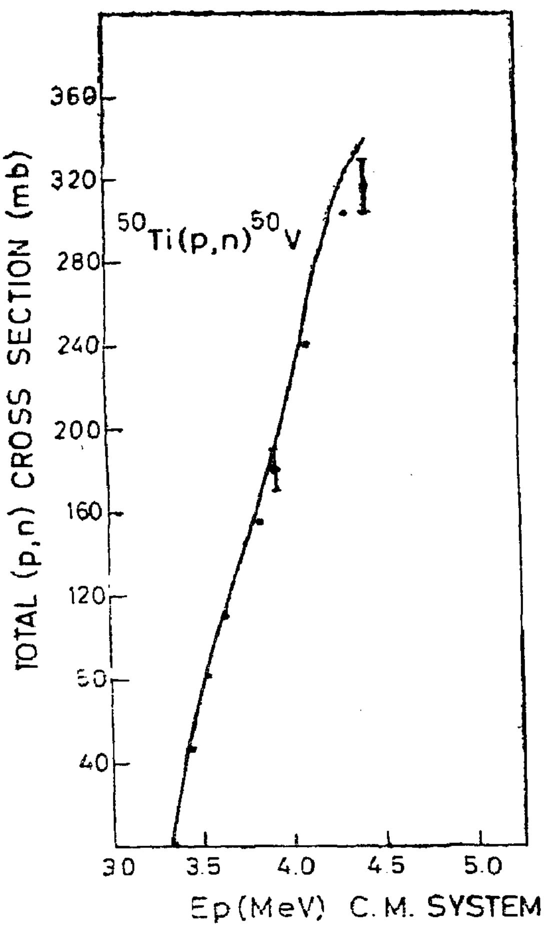

Figure 2. Averaged (p, n) excitation function for $^{50}Ti(p\ n)^{50}V$ reaction and the polynomial fit to the same. The observed threshold of this reaction is $c \sim 3 \cdot 4$ MeV.

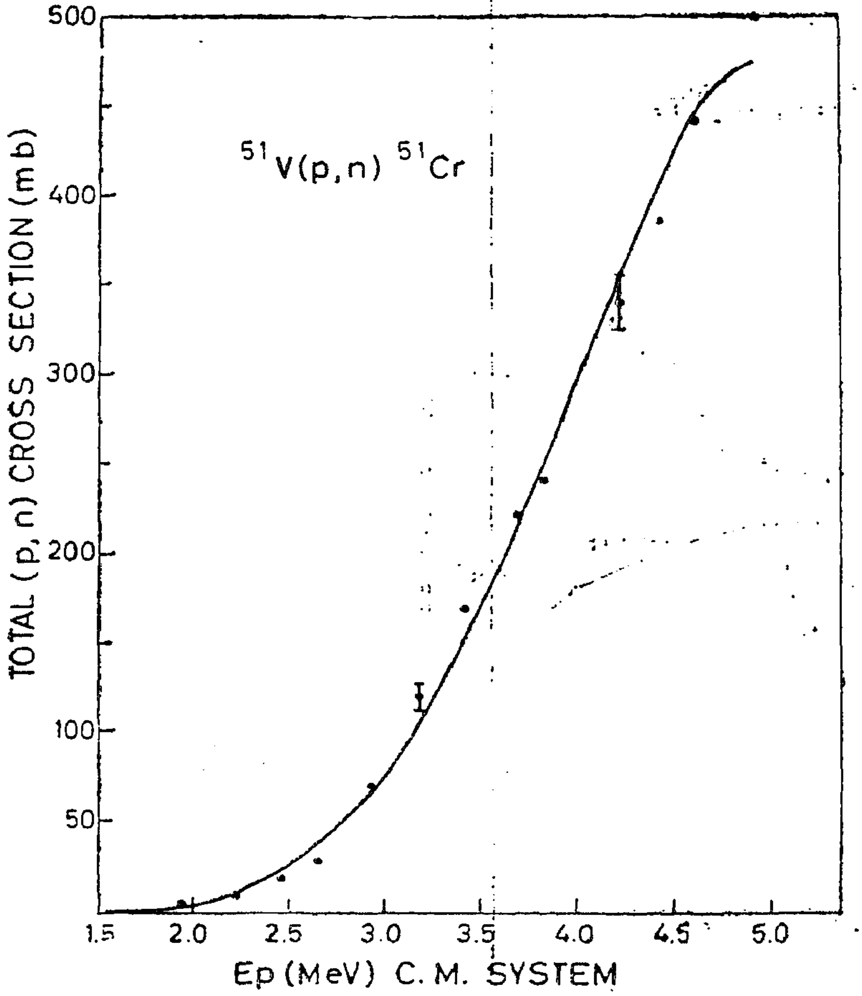

Figure 3. Averaged (p, n) excitation function for $^{51}V(p, n)^{51}Cr$ reaction and the polynomial fit to the same.

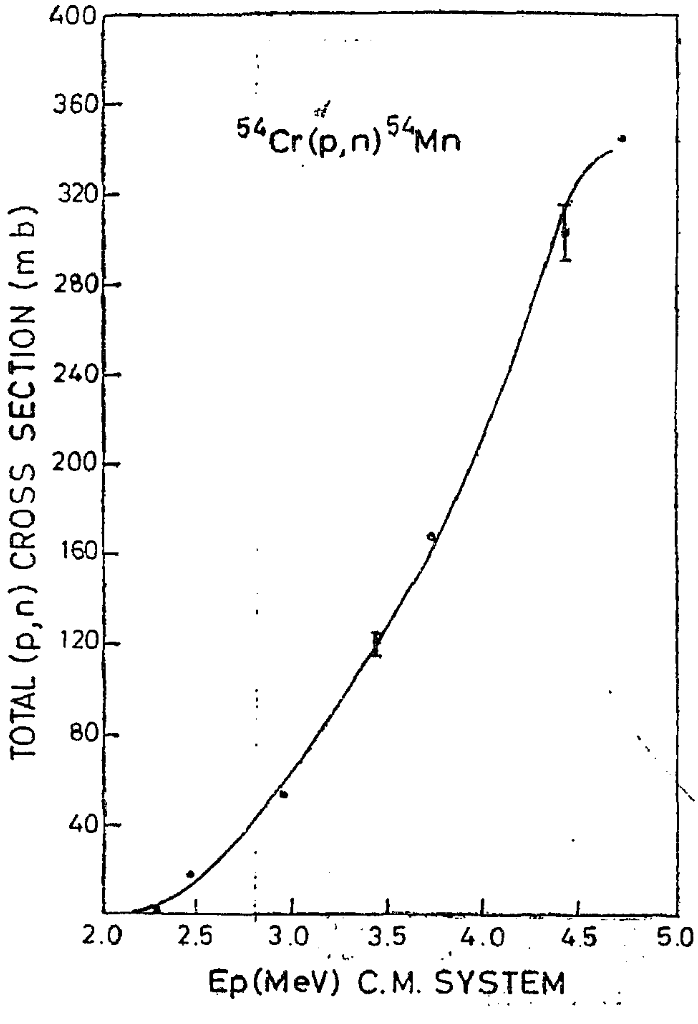

Figure 4. Averaged (p, n) excitation function for $^{54}Cr(p,n)^{54}Mn$ reaction and the polynomial fit to the same.

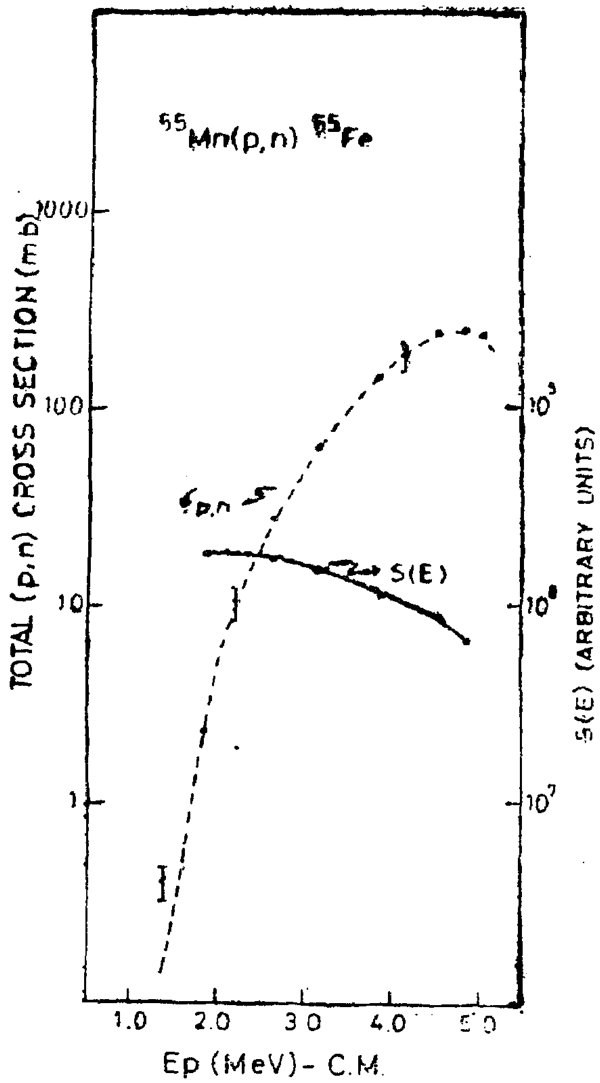

Figure 5. Averaged (p, n) excitation function for $^{55}Mn(p, n)^{55}Fe$ reaction and the polynomial fit to the same. The specific nuclear part of the interaction $S(E)$ is plotted as a function of energy.

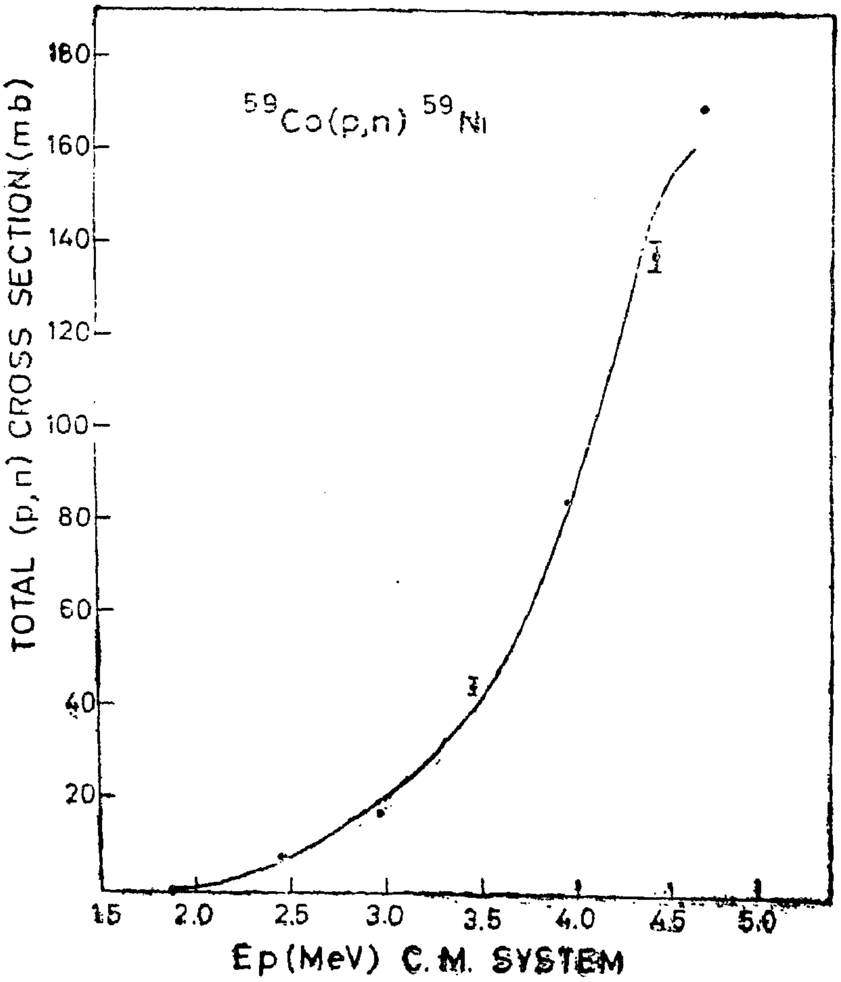

Figure 6. Averaged (p, n) excitation function for $^{59}Co(p,n)^{59}Ni$ reaction and the polynomial fit to the same.

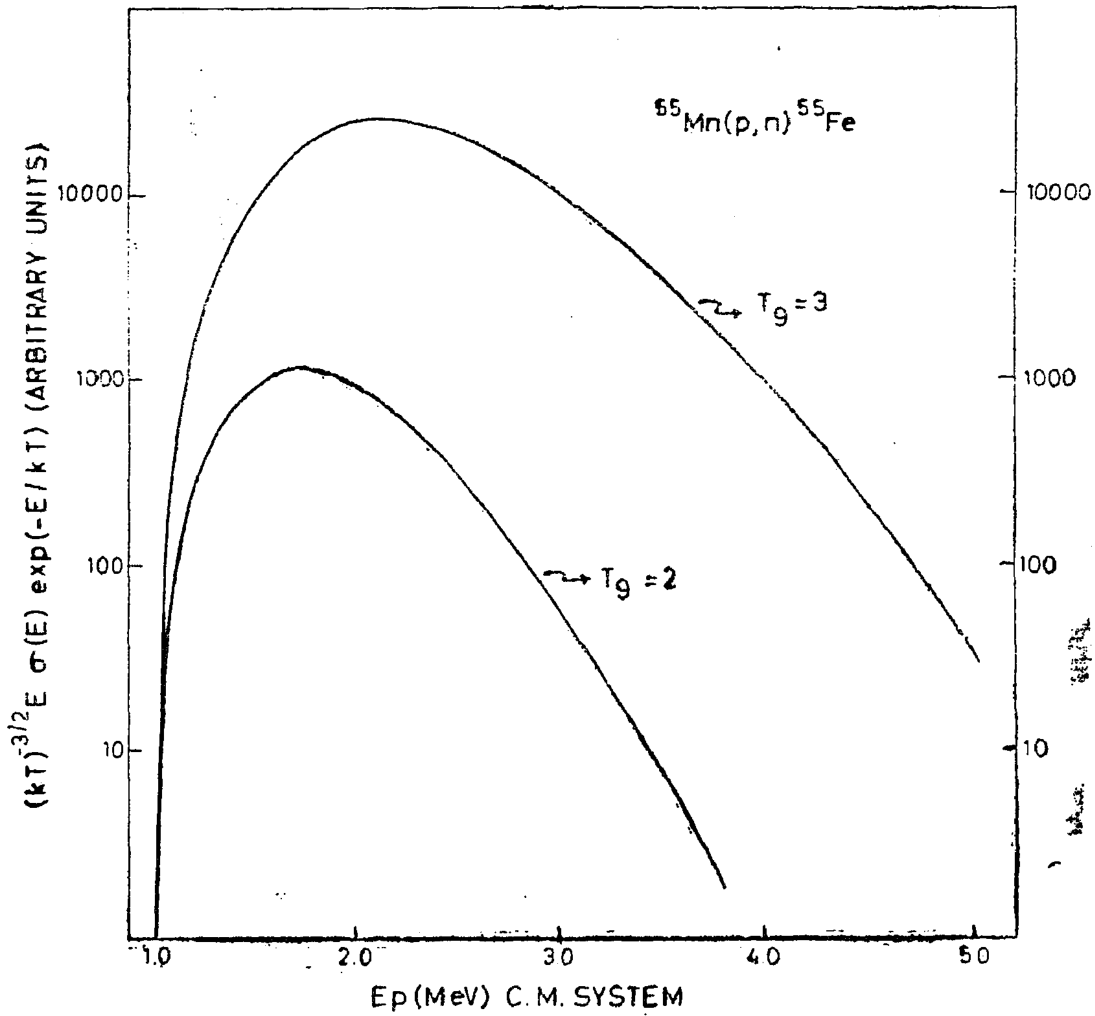

Figure 7. The integrant of the reaction rate expression (1) is plotted as a function of E for temperatures $T_9 = 2$ and 3.

to be accurate to within $\pm$ 25% ($\sim$ 20% error comes from $\sigma_{p,n}$ measurements). The TNRR values extracted at $T_9 = 3$, 5 from ^{45}Sc (p, n) ^{45}Ti are in fair agreement with the published values (Michaud and Fowler 1970).

Fowler (1973) has suggested that, as the reaction rates are used many times in calculations where the temperature is varied as a function of time, a standardised functional form would be more useful as a way of presenting reaction rates, than the listing of reaction rates at a few discrete temperatures. He has proposed that the equation

$$N_A \langle \sigma v \rangle = (P_1 + P_2 \, T_9{}^N) \exp\left(-\frac{|Q|}{kT}\right) \tag{10}$$

should govern the temperature dependence of the stellar reaction rates. Following the above-mentioned suggestion, the TNRR calculated for temperatures $T_9 = 1$ to 5 have been fitted to the above functional form using a non-linear least squares programme. The results of this analysis are also tabulated in table 1.

4. Conclusion

We have calculated here the thermonuclear (p, n) reaction rates in the temperature range $T_9 = 1$ to 5 for several medium weight nuclei from the experimentally

Table 1

Reaction	T_9 (10^9 °K)	E_0 (MeV)	ΔE (MeV)	$N_A\langle\sigma v\rangle$ $cm^3 g^{-1} sec^{-1}$	$N_A\langle\sigma v\rangle \exp\frac{\lvert Q\rvert}{kT_9}$ Experiment	$N_A\langle\sigma v\rangle \exp\frac{\lvert Q\rvert}{kT_9}$ Fit	P_1, P_2, N
$^{45}Sc(p,n)^{45}Ti$	1	0·922	0·651	4·7551 (−07)	9·3452 (+07)	1·0799 (+08)	..
$Q = -2·837$ MeV	2	1·463	1·161	9·7547 (+00)	1·3716 (+08)	1·2884 (+08)	9·646 (+07)
	3	1·918	1·627	2·8800 (+03)	1·6743 (+08)	1·5571 (+08)	1·153 (+07)
	4	2·323	2·068	5·1301 (+04)	1·9208 (+08)	1·8743 (+08)	1·49
	5	2·695	2·491	2·9235 (+05)	2·1115 (+08)	2·2331 (+08)	..
$^{50}Ti(p,n)^{50}V$	1	0·952	0·662	7·3284 (−09)	4·5435 (+08)	5·3103 (+08)	
	2	1·511	1·179	2·3259 (+00)	5·7914 (+08)	5·5883 (+08)	5·200 (+08)
$\lvert Q\rvert = 2·997$ MeV	3	1·979	1·653	1·6564 (+03)	6·5558 (+08)	6·0107 (+08)	1·104 (+07)
$Q_{eff} = -3·333$ MeV	4	2·398	2·101	4·3590 (+04)	6·8783 (+08)	6·5666 (+08)	1·815
	5	2·782	2·531	3·0090 (+05)	6·8691 (+08)	7·2491 (+08)	..
$^{51}V(p,n)^{51}Cr$	1	0·980	0·672	6·1859 (−02)	3·5503 (+06)	3·4047 (+06)	..
$Q = -1·540$ MeV	2	1·556	1·197	1·0475 (+03)	7·9357 (+06)	8·2554 (+06)	2·136 (+06)
	3	2·039	1·678	4·3955 (+04)	1·6955 (+07)	1·7496 (+07)	1·269 (+06)
	4	2·470	2·133	3·6684 (+05)	3·1929 (+07)	3·1645 (+07)	2·270
	5	2·866	2·569	1·4760 (+06)	5·2585 (+07)	5·1104 (+07)	..

Table 1 (*Contd.*)

$^{54}Cr(p,n)^{54}Mn$	1	1·009	0·682	2·4421 (−04)	1·8634 (+07)	1·8770 (+07)	..
$Q = -2{\cdot}160$ MeV	2	1·602	1·214	1·5924 (+02)	4·3987 (+07)	4·3740 (+07)	1·747 (+06)
	3	2·099	1·703	1·7321 (+04)	7·3467 (+07)	7·2959 (+07)	1·702 (+07)
	4	2·542	2·164	2·0148 (+05)	1·0589 (+08)	1·0533 (+08)	1·303
	5	2·950	2·606	9·2368 (+05)	1·3869 (+08)	1·4028 (+08)	..
$^{55}Mn(p,n)^{55}Fe$	1	1·037	0·691	3·5123 (−01)	4·4083 (+04)	4·3862 (+04)	..
	2	1·646	1·231	1·1469 (+03)	4·0632 (+05)	4·2458 (+05)	8·125 (+03)
$Q = -1{\cdot}012$ MeV	3	2·157	1·726	3·5688 (+04)	1·7867 (+06)	1·7596 (+06)	3·574 (+04)
	4	2·613	2·194	2·6591 (+05)	5·0050 (+06)	4·8612 (+06)	3·543
	5	3·032	2·642	1·0052 (+06)	1·0519 (+07)	1·0707 (+07)	..
$^{59}Co(p,n)^{59}Ni$	1	1·092	0·709	1·1040 (−03)	2·8468 (+06)	2·9020 (+06)	..
	2	1·733	1·263	1·3348 (+02)	6·7782 (+06)	6·5910 (+06)	1·514 (+06)
$Q = -1{\cdot}858$ MeV	3	2·271	1·771	9·1083 (+03)	1·2490 (+07)	1·2355 (+07)	1·388 (+06)
	4	2·751	2·251	8·9244 (+04)	2·0111 (+07)	2·0086 (+07)	1·871
	5	3·193	2·711	3·8365 (+05)	2·9256 (+07)	2·9710 (+07)	..

measured reaction cross sections below 5 MeV bombarding energy. These are of astrophysical importance, particularly in the study of nucleosynthesis of mass around 56. It is evident from table 1, that the functional form suggested by Fowler is reasonably good in explaining the temperature dependence of the reaction rates.

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