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ENHANCEMENT OF NUCLEOSYNTHESIS REACTION RATES DUE TO NONTHERMALIZED FAST NEUTRONS

YU. V. PETROV AND A. I. SHLYAKHTER
Leningrad Nuclear Physics Institute
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ABSTRACT

It is usually assumed in stellar nucleosynthesis calculations that neutrons are completely thermalized. Hence, if the cross section of a neutron-induced reaction has a threshold, or it is suppressed by the Coulomb barrier in the exit channel, the reaction rate is quite low. However, the contribution from the decelerating fast neutrons has been neglected previously. We show that, though the fraction of such neutrons is small, they enhance a number of nucleosynthesis reaction rates by many orders of magnitude, especially at low temperatures.

Subject headings: nucleosynthesis

I. INTRODUCTION

Stellar neutrons are produced mainly in (α, n) reactions, e.g., in $^{13}C(\alpha, n)\ ^{16}O$ and $^{22}Ne(\alpha, n)\ ^{25}Mg$ (Mathews and Ward 1985). Their initial energies vary from 0.1 MeV to several MeV depending on the particular source and the surrounding temperature. It is usually assumed that neutrons are immediately slowed down and thermalized, so that one can average their cross sections over the Maxwell spectrum (Allen, Gibbons, and Macklin 1971; Woosley *et al.* 1978, hereafter WFHZ78). The fraction of the epithermal neutrons (γ—the "hardness" of the neutron spectrum) can be easily estimated from the balance between the decelerating[1] neutrons and those captured in the thermal region:

$$\gamma = \frac{\phi_f}{\phi_{th}} = \frac{\sum_a}{\xi \sum_s}, \quad \xi = 1 + \frac{\epsilon \ln \epsilon}{1 - \epsilon}, \quad \epsilon = \left(\frac{A-1}{A+1}\right)^2 . \quad (1)$$

Here $\phi_f = \langle n_n v \rangle_f$ and $\phi_{th} = \langle n_n v \rangle_{th}$ are the fluxes of the epithermal and thermal neutrons, respectively, ξ is the mean change of the lethargy u [$u = \ln (E^*/E)$, $E^* \equiv 2$ MeV] in a single collision, A is the atomic weight of the moderator, $\sum_a$ and $\sum_s$ are the mean macroscopic capture and scattering cross sections and $\xi \sum_s$ is the "slowing down" cross section ($\sum_a = \sum_i n_i \sigma_{ai}$, $\sum_s = \sum_i n_i \sigma_{si}$, $\xi \sum_s = \sum_i n_i \xi_i \sigma_{si}$, n_i is the number density of the ith nuclide, σ_{ai} and σ_{si} are its capture and scattering cross sections).

Usually γ is quite small. Let us accept for the s-process the abundances in the helium layer of a red giant calculated by Iben 1975 (95% ^4He, 5% ^{12}C, 0.4% ^{22}Ne, and heavies after many flashes) and the solar values (from Cameron 1982) for the abundances of nuclides up to ^{58}Fe (except the CNO nuclides which are transformed into ^{22}Ne). Then neutrons are slowed down mainly due to their scattering on ^4He ($\xi = 0.425$, $\sigma_s \approx 1b$). Using data from Almeida and Käppeler 1983, one obtains the effective capture cross section of stellar substance $\sigma_a \approx 1.5$ mb and equation (1) gives $\gamma \approx 10^{-5}$. To an order of magnitude this estimate is also valid for the ^{13}C neutron source. A similar estimate for the typical abundances of nuclides at the advanced burning stages—47% ^{16}O, 25% ^{12}C, 25% ^{20}Ne, 3% ^{24}Mg, 0.2% ^{28}Si (1.7–6 $M_\odot$ mass zone of the 25 $M_\odot$ presupernova model of Woosley and Weaver 1982)—gives $\gamma \approx 10^{-3}$.

Our basic idea is that even for such small values of γ, the contribution of fast neutrons can be important if the reaction cross section has a high threshold $|Q| \gg kT$ or if it is suppressed by the Coulomb barrier in the exit channel. Usually only the exponentially small fraction of fast neutrons in the Maxwell spectrum was taken into account in the calculations of the rates of these reactions. Here we take into account the contribution of the decelerating neutrons and show that in a number of cases it enhances the neutron reaction rates by many orders of magnitude, especially at low temperatures.

II. THE NEUTRON SPECTRUM

The spectrum of neutrons produced in a binary thermonuclear reaction, in which the particles 1 and 2 collide with the center-of-mass energy ϵ and produce the particle 3 and the neutron, was obtained by Williams 1971 (see his eq. [48]). His result can be presented in the form

$$f(E) = \frac{2.65 \times 10^8}{N_A \langle \sigma v \rangle T^2} \frac{A}{(\lambda A_1 A_2)^{1/2}} \int_0^\infty d\epsilon \frac{\epsilon \sigma(\epsilon)}{(\epsilon + Q)^{1/2}} \times e^{-\{\epsilon + A[E + \lambda(\epsilon + Q)]\}/T} sh \frac{2A}{T} [\lambda E(\epsilon + Q)]^{1/2} ,$$

$$A = A_1 + A_2, \qquad \lambda = 1 - 1/A . \quad (2)$$

Here $T = T_9/11.605$ is the thermal energy in MeV (T_9 is the temperature, 10^9 K), A_i is the atomic weight of the ith nuclide, $\sigma(\epsilon)$ is the reaction cross section (in barns). Note that for threshold reactions ($Q < 0$) $\sigma(\epsilon) = 0$ if $\epsilon + Q \le 0$. Integrating $f(E)$ over E gives the usual formula for the total rate of neutron production (WFHZ78):

$$N_A \langle \sigma v \rangle = \frac{9.40 \times 10^8}{(T^3)^{1/2}} \left(\frac{A}{A_1 A_2}\right)^{1/2} \times \int_0^\infty d\epsilon \epsilon \sigma(\epsilon) e^{-\epsilon/T} \text{ cm}^3 \text{ s}^{-1} \text{ mole}^{-1} . \quad (3)$$

If $A \gg 1$ the neutron carries away nearly all available energy $\epsilon + Q$. This follows from equation (2) where the integrand has a sharp peak near $\epsilon = E/\lambda - Q$. Using the nonresonant form of

[1] Let us note that in the physics of nuclear reactors the term "slowing down" is used in place of "deceleration" (Weinberg and Wigner 1959). The lethargy u is a convenient variable since the number of collisions decelerating a neutron down to the energy E is proportional to $\ln (E^{-1})$.

the cross section,

$$\sigma(\epsilon) = \frac{S(\epsilon)}{\epsilon} e^{-b/(\epsilon)^{1/2}} , \qquad (4)$$

where the factor $S(\epsilon) = 0$ if $\epsilon + Q \le 0$ and varies slowly if $\epsilon + Q > 0$. Evaluating the integral by the method of steepest descent we obtain the approximate energy spectrum of the neutron source:

$$f(E) = \frac{9.40 \times 10^8}{(T^3)^{1/2}} \left(\frac{A}{A_1 A_2}\right)^{1/2} S(\epsilon_0) e^{-b/(\epsilon_0)^{1/2} - \epsilon_0/T} \text{ MeV}^{-1} , \qquad (5)$$
$$\epsilon_0 = E/\lambda - Q .$$

Here $b = (E_G)^{1/2} = 0.9895\, Z_1 Z_2 [A/(A_1 A_2)]^{1/2}$ MeV$^{1/2}$, where E_G is the Gamow energy, $E_G = (2\pi\alpha Z_1 Z_2)^2 Mc^2/2$, α is the fine structure constant, c is the speed of light, Z_1 and Z_2 are the charges of the colliding particles and M is the reduced mass. The $S(\epsilon)$ factor is in units of MeV barns. It follows from equation (5) that most of the neutrons are born with the energies near E_0:

$$E_0 = \lambda \left\{ \left[\frac{b}{2(1/T + B)}\right]^{2/3} + Q \right\} , \qquad (6)$$

where the parameterization $S(\epsilon) = S_r \exp(-B\epsilon)$ is used. Near E_0 the spectrum can be approximated by a Gaussian

$$f(E) = \frac{1}{(2\pi)^{1/2}\Gamma} \exp\left[-\frac{(E - E_0)^2}{2\Gamma^2}\right]$$
$$= \frac{2^{1/6}\lambda}{3^{1/2}} \frac{b^{1/3}}{(1/T + B)^{5/6}} . \qquad (7)$$

If the inelastic scattering, and absorption of fast neutrons, as well as the Placzek oscillations (see, e.g., Weinberg and Wigner 1959), can be neglected, then the neutron spectrum is described by the sum of two spectra: the spectrum of the source plus the Fermi spectrum of the decelerating neutrons.

$$\phi(E) = f(E) + \frac{1}{\xi \sum_s E} \int_E^\infty f(\epsilon) d\epsilon , \qquad (8)$$

where $\phi(E)$ is the neutron flux (in cm^{-2} s^{-1}).

The fraction of nonthermalized neutrons is small at thermal energies; therefore, the Maxwell spectrum is a good approximation. At high energies both the unscattered neutrons coming directly from the source and the decelerating neutrons may make the main contribution. The intermediate energy range also exists of course, but since the absorption is small it can be replaced by an effective matching energy E_c (which is a conventional procedure used in the physics of nuclear reactors; see, e.g., Galanin 1984). We have

$$\phi(E) = \phi_{\text{th}} E/T^2 e^{-E/T} \qquad \text{at } E \le E_c ,$$
$$\phi(E) = f(E)/\textstyle\sum_s + \frac{1}{\xi \sum_s E} \int_E^\infty f(\epsilon) d\epsilon \quad \text{at } E > E_c . \qquad (9)$$

The matching point is determined by the balance between the neutrons absorbed at $E \leqslant E_c$ and the total number of neutrons produced.

Assuming that (1) $E_c \gg T$, (2) the capture cross section follows the "$1/v$" law, and (3) the influence of the capture of neutrons on their deceleration is negligible, one obtains the absorption rate $(\pi^{1/2}/2) \sum_a(T)\phi_{\text{th}}$, so that $\sum_s \phi_{\text{th}} = 2/(\pi)^{1/2}(\gamma\xi)^{-1}$ (the spectrum of the source is normalized to 1 neutron s^{-1} cm^{-3}). Introducing the collision density $F = \phi \sum_s$ we finally obtain

$$F(E) = \begin{cases} \dfrac{2}{\pi^{1/2}} \dfrac{1}{\gamma\xi} \dfrac{E}{T^2} e^{-E/T} , & E \le E_c , \\ f(E) + \dfrac{1}{\xi E} \displaystyle\int_E^\infty f(\epsilon) d\epsilon , & E > E_c . \end{cases} \qquad (10)$$

In agreement with the estimate of § I, the fraction of fast neutrons is of the order of γ. In the computer calculations $F(E)$ is first determined in the high-energy region and then extrapolated downward, until at E_c it becomes equal to the Maxwell spectrum which is used at $E \le E_c$. The resulting spectra for ^{13}C and ^{22}Ne sources at $T_9 = 0.3$, with pure ^{4}He as the moderator ($\xi = 0.425$), and $\gamma = 10^{-3}$ are shown in Figure 1. In the region $E > 0.6$ MeV the spectrum is completely determined by the decelerating neutrons. In the ^{22}Ne case the spectrum decreases quickly because E_0 is rather small ($E_0 = 0.11$ MeV, while for ^{13}C, $E_0 = 2.49$ MeV).

To summarize, we have shown that the high-energy part of the neutron spectrum is mainly due not to the tail of the Maxwell distribution, but to decelerating fast neutrons.

III. RATES OF (n, p), (n, α), AND (n, n') REACTIONS INCLUDING FAST NEUTRONS

In previous sections we have used the neutron flux $\phi(E)$ for the description of the spectra. The reaction rate is then given by the product $\langle\sigma\rangle\langle\phi\rangle$. However, in the nucleosynthesis calculations it is the neutron density that is known, while $\langle\sigma v\rangle n$ should be determined. For this reason, here we shall use the cross sections averaged over the neutron energy distribution $n(E) = \phi(E)/v(E)$ instead of those averaged over $\phi(E)$:

$$N_A\langle\sigma_r v\rangle = N_A \frac{\int_0^\infty dE \sigma_r(E) v(E) n(E)}{\int_0^\infty dE n(E)} . \qquad (11)$$

The main contribution in the denominator comes from thermal neutrons. The integral over the Maxwell spectrum gives $(\gamma\xi v_{\text{th}})^{-1}$, and we obtain

$$N_A\langle\sigma_r v\rangle_{\text{th}} = \frac{2}{\pi^{1/2}} N_A v_{\text{th}} \int_0^\infty dE \sigma_r(E) E/T^2 e^{-E/T} . \qquad (12)$$

Here v_{th} and E are the thermal velocity and the energy of the neutron in the center-of-mass system ($T \equiv E_{\text{th}}$). If the value of $\sigma_r(E)$ is appreciable only at $E \gg T$, the contribution of thermal neutrons is exponentially small and the reaction rate is determined by the integral over the spectrum of fast neutrons:

$$N_A\langle\sigma_r v\rangle_f = \gamma\xi N_A v_{\text{th}} \int_{E_c}^\infty dE \sigma_r(E) \left[f(E) + \frac{1}{\xi E} \int_E^\infty d\epsilon f(\epsilon) \right] . \qquad (13)$$

In order to estimate this integral, we shall neglect the dispersion of the energies of produced neutrons by replacing $f(E)$ by the delta function $\delta(E - E_0)$. Using for the (n, p) and (n, α) cross sections the parameterization similar to equation (4) and assuming that $A \gg 1$ one has

$$N_A\langle\sigma_r v\rangle_f = \gamma\xi N_A v_{\text{th}} S_r \left[\frac{e^{-b_r/E_0^*}}{E_0} + \frac{1}{\xi} \int_0^{E_0} \frac{e^{-b_r/(E^*)^{1/2}}}{E^2} dE \right] , \qquad (14)$$
$$E^* = E + Q_r .$$

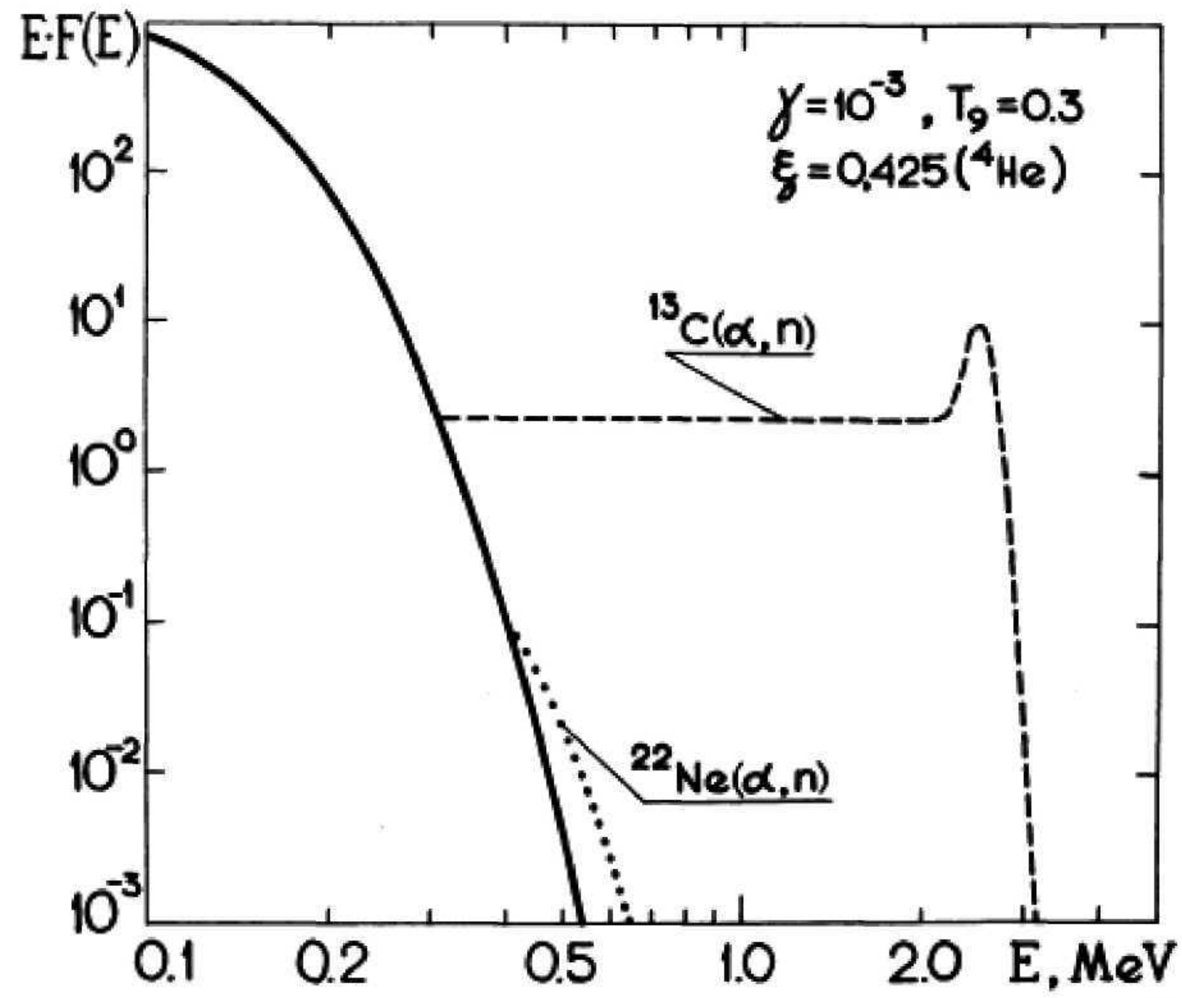

FIG. 1.—Neutron spectrum $E\,F(E)$ calculated using eqs. (2) and (10) and showing the following: Maxwell spectrum (*solid line*); ^{13}C(α, n) source ($Q_{\alpha n} = 2.215$ MeV) (*dashed line*); ^{22}Ne(α, n) source ($Q_{\alpha n} = -0.48$ MeV) (*dotted line*).

The main contribution to the integral comes from the high-energy region. Neglecting the E dependence of the slowly varying terms we finally obtain

$$N_A\langle\sigma_r v\rangle_f = 2.44 \times 10^8 \gamma\xi(T_9)^{1/2}\sigma_r(E_0) \times \left(1 + \frac{2[(E_0^*)^3]^{1/2}}{\xi b_r E_0}\right) \text{cm}^3\ \text{s}^{-1}\ \text{mole}^{-1}\ . \quad (15)$$

Here the cross section σ_r is in barns. It follows from equation (6) that for $Q_{\alpha n} > 0$ the value of E_0 and, hence, the reaction rate depend on the temperature rather weakly. Thus, although the fraction of epithermal neutrons is small, at moderate temperatures their contribution is the main one. Note that if the cross section $\sigma_r(E)$ has a resonance near E_0 the reaction rate can be further enhanced. The contribution of the reactions occurring on the excited states is usually small and is neglected here for simplicity, but it can be taken into account by averaging equation (15) over the level populations.

A similar approximation can be easily obtained for the inelastic excitation of nuclear levels by fast neutrons:

$$N_A\langle\sigma_{nn'}v\rangle_f = 2.44 \times 10^8\ \gamma\xi(T_9)^{1/2} \times \left[\sigma_{nn'}(E_0) + \frac{1}{\xi}\int_{\epsilon_l}^{E}\frac{d\epsilon}{\epsilon}\,\sigma_{nn'}(\epsilon)\right]\text{cm}^3\ \text{s}^{-1}\ \text{mole}^{-1} \quad (16)$$

where ϵ_l is the level energy.

Table 1 displays the results of numerical integration of the ^{40}Ca(n, p) ^{40}K ($Q_{np} = -0.529$ MeV) cross section using the exact neutron spectrum of the source (eqs. [2], [12], [13]). The cross section $\sigma_{np}(E)$ was calculated using the Hauser-Feshbach-type formulae (Woosley and Fowler 1977; WFHZ78) with the help of the CINDY code (Sheldon and Rogers 1973) which was modified to deal with the square well optical model potential. The Coulomb wave functions were computed using the RCWFN code (Barnett *et al.* 1974). In the

TABLE 1

REACTION RATE $N_A\langle\sigma_{np}v\rangle$ cm^3 s^{-1} mole^{-1} FOR ^{40}Ca(n, p) ^{40}K

	$\gamma=0$		$\gamma=10^{-5}$		$\gamma=10^{-3}$	
T_9	WFHZ75	This Paper	^{22}Ne(α, n)	^{13}C(α, n)	^{22}Ne(α, n)	^{13}C(α, n)
0.1	2.5(−39)	2.4(−39)	9.2(−39)	2.7(+1)	9.2(−37)	2.7(+3)
0.3	4.8(−13)	5.2(−13)	5.8(−12)	7.7(+1)	5.8(−10)	7.7(+3)
0.5	1.7(−6)	1.8(−6)	5.7(−6)	1.4(+2)	5.6(−4)	1.4(+4)
1	1.3	1.3	1.3	3.7(+2)	1.8(+1)	3.7(+4)
2	6.2(+3)	6.1(+3)	6.1(+3)	6.7(+3)	7.1(+3)	9.1(+4)
3	1.9(+5)	1.8(+5)	1.8(+5)	1.8(+5)	1.8(+5)	2.9(+5)

NOTE.—Parentheses indicate multiplication by the power of 10 specified within the parentheses.

$\gamma = 0$ case which describes the purely thermal neutron spectrum, the reaction rate calculated by Woosley *et al.* (1975, hereafter WFHZ75) is also listed. The discrepancy does not exceed 10% and is probably due to the different treatment of continuum levels. The contribution of fast neutrons is shown for two neutron sources: ^{22}Ne(α, n) ^{25}Mg ($Q_{\alpha n} = -0.48$ MeV) and ^{13}C(α, n) ^{16}O ($Q_{\alpha n} = 2.215$ MeV). It is assumed that $\gamma = 10^{-3}$ and pure ^{4}He is a moderator ($\xi = 0.425$). The values of the parameter B in equations (5) and (6) are 0.636 MeV^{-1} for ^{22}Ne (Ashery 1969) and -2.2 MeV^{-1} for ^{13}C (Davids 1968). It is evident from Table 1 that, at low temperatures, fast neutrons enhance the reaction rate by many orders of magnitude.

Using the simplified equation (15) one can easily obtain the reaction rates for any stellar composition described by the two parameters γ and ξ. For example, let us consider the ^{13}C source at $T_9 = 0.3$. Equation (6) gives $E_0 = 2.46$ MeV ($b_{\alpha n} =$ 20.77 MeV$^{1/2}$). For the ^{40}Ca(n, p) ^{40}K reaction ($b_{np} = 18.57$ MeV$^{1/2}$, σ_{np} (2.5 MeV) = 0.09 b(WFHZ75); equation (14) gives $E_0^* = 1.96$ MeV. Substituting these values into equation (16), one finds that at $\gamma = 10^{-5}$, $\xi = 0.425$ $N_A\langle\sigma_{np}v\rangle = 6.5 \times 10^1$ cm^3 s^{-1} mole^{-1}, which is 20% less than the rate obtained by numerical integration. Such an accuracy is quite sufficient since the optical model calculations with the global potential give the cross section only within a factor of 2 (see, e.g., WFHZ78 and Bartle *et al.* 1974, 1981). Note that for the endothermic source ^{22}Ne, the relative dispersion in the energies of the produced neutrons is not small, so that equation (15) is inapplicable and a numerical calculation is required. However, as can be seen from Table 1, the enhancement of the reaction rate for this source is far less than that for ^{13}C.

Besides using it for the case of the ^{40}Ca(n, p) ^{40}K reaction, we have used equation (15) to estimate the rates of the six reactions considered in nucleosynthesis calculations (Howard *et al.* 1972; Clayton and Woosley 1974; Busso and Gallino 1985), ^{36}Ar(n, p) ^{36}Cl, ^{38}Ar(n, p) ^{38}Cl, ^{38}Ar(n, α) ^{35}S, ^{50}Cr(n, p) ^{50}V, ^{54}Fe(n, p) ^{54}Mn, and ^{58}Ni(n, p) ^{58}Fe for three exothermic sources: ^{13}C(α, n) ^{16}O, ^{21}Ne(α, n) ^{24}Mg, and ^{25}Mg(α, n) ^{28}Si. Just as in the ^{40}Ca case the comparison with the calculation for thermalized neutrons (WFHZ75) shows that fast neutrons enhance the reaction rates by many orders of magnitude.

IV. SUMMARY

It is shown that under stellar conditions the main contribution to the rates of (n, p), (n, α), and (n, n') reactions may be due to decelerating fast neutrons. Taking this contribution into account enhances the rates of a number of nucleosynthesis reactions by many orders of magnitude, especially at low temperatures. The importance of fast neutrons depends on their initial energy E_0 and nuclide abundances in the stellar substance which define the spectrum hardness γ. This dependence opens an essentially new way of testing the nucleosynthesis models using "stellar dosimeters," i.e., nuclides, the abundances of which are sensitive to the spectrum of decelerating neutrons.

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YU. V. PETROV AND A. I. SHLYAKHTER: Leningrad Nuclear Physics Institute, Gatchina, Leningrad 188350, USSR