

PRODUCTION OF HEAVY ELEMENTS IN INHOMOGENEOUS COSMOLOGIES

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ABSTRACT

Baryon density inhomogeneities during big bang nucleosynthesis can result from a variety of possible causes (e.g., quantum chromodynamic and electroweak phase transitions; cosmic strings). We present here the consequences of such inhomogeneities with special emphasis on the production of *heavy* elements in a parameter study, varying the global baryon-to-photon ratio η [which is related to the baryon density and the Hubble constant via $\eta_{10} = 64.94\Omega_b(H_0/50)^2$] and the length scale of the density inhomogeneities. The production of heavy elements beyond Fe can only occur in neutron-rich environments; thus, we limit our study to neutron-rich zones, originating from neutron diffusion into low-density regions. In this first calculation including elements heavier than Si, we prove an earlier hypothesis that under such conditions *r*-process elements can be produced, strongly enhanced by the process of fission cycling. Primordial *r*-process abundances are, however, very sensitive to the choice of η . Significant amounts, comparable to or larger than the (permitted) floor of heavy-element abundances found in low-metallicity stars at the onset of galactic evolution, can only be obtained for values in excess of $\eta_{10} = 133$ (i.e., $\Omega_b h_{50}^2 = 2.0$; e.g., $\Omega_b = 1$, $H_0 = 71$ or $\Omega_b = 0.5$, $H_0 = 100$) and large length scales of inhomogeneities, which minimize the back-diffusion of neutrons into proton-rich regions. Recent investigations analyzing the primordial abundances of light elements seem to set tighter limits, $\eta_{10} < 26$ – 39 ($\Omega_b h_{50}^2 < 0.4$ – 0.6), from ${}^4\text{He}$ and apparently considerably lower values based on Li, Be, and B. Under such conditions the predicted abundances of heavy elements are a factor of 10^5 or more below presently observable limits.

Subject headings: diffusion — early universe — nuclear reactions, nucleosynthesis, abundances

1. INTRODUCTION

The application of the gauge theories of particle physics to big bang cosmology strongly suggests that the universe underwent several phase transitions during its early evolution. In the standard model the temperature interval between roughly 1 TeV and 100 MeV is rich in physical phenomena: electroweak symmetry breaking, chiral symmetry breaking, and quark confinement all occur in this interval. A first-order phase transition can render the baryon distribution of an initially homogeneous universe quite inhomogeneous, and inhomogeneities generated during or after the electroweak transition can survive until primordial nucleosynthesis and affect the abundances of the isotopes produced in the big bang. The possibility that the changes in the abundance pattern might be drastic enough to reconcile a closure density of baryons with primordial nucleosynthesis constraints, or to produce a characteristic signature of a phase transition in the early universe, has proved exciting enough to inspire a considerable amount of work on inhomogeneous nucleosynthesis.

It is now generally agreed that a closure density of baryons cannot be reconciled with the light-element abundances in any straightforward manner, but the possibility of detecting the handiwork of phase transitions remains (see Malaney & Mathews 1993).

In this paper we analyze one of the proposed signatures of inhomogeneity, the synthesis of very heavy elements by neutron capture. We find that heavy elements (the *r*- and *s*-process elements of stellar nucleosynthesis) can be produced in observable, and sometimes excessive, quantities in models with mean baryon densities near closure, large Hubble constants, and large length scales for the inhomogeneities. We find that the heavy-element production is very sensitive to baryon density. The heavy-element abundances in models with mean baryon densities of a few percent of closure and small Hubble constants are several orders of magnitude below current observational limits to the primordial heavy-element abundance.

The richness of cosmological scenarios involving first-order phase transitions occurring in or near equilibrium was first pointed out by Witten (1984) in the context of the quark confinement transition in quantum chromodynamics (QCD). Witten realized that baryon number would be concentrated in

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the quark phase if baryon chemical equilibrium could be established, and that the transport of baryon number at the phase boundary was such that baryon number concentration could occur even if complete chemical equilibrium could not be established. This led him to predict that large-amplitude baryon density inhomogeneities could be produced in the QCD phase transition, and to speculate that if bulk strange quark matter were the true ground state of strongly interacting matter, then nuggets of quark matter could be produced in the early universe and survive today as the dark matter in the universe. In the simplest version of this scenario a few percent of the baryon number remained as protons and neutrons in the gas phase, and the rest ended up in nuggets of strange quark matter. This allowed a closure density of a single type of particle, which was attractive from an aesthetic point of view. Subsequent work (Applegate & Hogan 1985; Alcock & Farhi 1985; Madsen, Heislerberg, & Rijsager 1986; Alcock & Olinto 1989; Madsen & Olesen 1991) has shown that the strength of the baryon number concentration was overestimated in Witten's paper and that quark matter nuggets are not attractive dark matter candidates. However, Witten's paper remains important because the production of density inhomogeneities is a generic feature of the QCD transition, and this feature underlies all of the later work on the effect that the QCD transition may have had on primordial nucleosynthesis.

It was quickly realized (Applegate & Hogan 1985; Bonometto, Marchetti, & Matarrese 1985; Sale & Mathews 1986) that the inhomogeneities predicted by Witten would have consequences for primordial nucleosynthesis. In particular, Applegate & Hogan (1985) realized that the inhomogeneities produced in the QCD transition could give rise to a very rich set of scenarios for primordial nucleosynthesis. The most interesting of the effects they discussed is the differential diffusion of neutrons and protons. The neutron, being electrically neutral, has a mean free path roughly a factor of 10^6 times that of the proton. Neutrons can diffuse to uniformity over much larger distances than protons. This has the effect of converting density variations into variations of the local neutron-to-proton ratio and, if the density variations are of sufficiently large amplitude, producing local environments in which neutrons outnumber protons. Nucleosynthesis in universes with both neutron-rich and proton-rich environments can be much different from that in the standard homogeneous, proton-rich big bang. The possibilities ranged from ruling out Witten's scenario, to detecting the handiwork of the cosmological QCD transition, to possibly matching the success of the standard model in predicting the abundances of the light elements in a model with a closure density of baryons.

These exciting possibilities led to the study of neutron diffusion and light-element nucleosynthesis in the early universe by many authors (Applegate, Hogan, & Scherrer 1987, 1988; Alcock, Fuller, & Mathews 1987; Fuller, Mathews, & Alcock 1988; Malaney & Fowler 1988; Kurki-Suonio et al. 1988; Kurki-Suonio & Matzner 1989; Kurki-Suonio et al. 1990; Terasawa & Sato 1989a, b, c; Mathews et al. 1988; Mathews, Alcock, & Fuller 1990; Mathews, Boyd, & Fuller 1993a; Mathews, Schramm, & Meyer 1993b; see the review by Malaney & Mathews 1993). Nucleosynthesis in a universe that has both neutron- and proton-rich regions will produce more ^2H , less ^4He , and more ^7Li than a homogeneous, proton-rich universe with the same global value of the baryon density. The majority of the debate in this field has centered on the question of whether the closure density inhomogeneous models could

avoid overproducing ^4He and ^7Li . The details of this debate, particularly the discussion of the subtle and complicated astrophysical issues involved in the destruction of ^7Li in stars, are beyond the scope of this paper. The present consensus in the field is that the light-element abundances cannot be fitted with any inhomogeneous model with a closure density of baryons, and that these models are ruled out by the data (see Ryan et al. 1992 and Duncan, Lambert, & Lemke 1993 for observations of B and Be abundances).

One of the signatures of nucleosynthesis in neutron-rich environments is the production of heavy elements. The absence of a Coulomb barrier allows neutrons to induce reactions long after all charged particle reactions have frozen out. In the standard model, neutrons are consumed rapidly by the production of ^4He , so there are none left by the time the charged particle reactions have frozen out. The neutron-rich regions in the inhomogeneous models have a surplus of neutrons at late times, so low-temperature (n, γ) nucleosynthesis is possible. The first calculations of nucleosynthesis under neutron-rich conditions (Applegate et al. 1987; Alcock et al. 1987; Malaney & Fowler 1988) found that the abundances of the isotopes of carbon and heavier nuclei (most of which was ^{14}C) were orders of magnitude higher than in proton-rich environments with the same baryon density. Later, Applegate (1988) and Applegate et al. (1988) found that once ^{18}O is produced by the $^{14}\text{C}(\alpha, \gamma)^{18}\text{O}$ reaction, much heavier elements could be produced by sequences of neutron captures and beta decays. Kajino, Mathews, & Fuller (1990) treated nuclei as heavy as Si in their calculations.

Neutron capture nucleosynthesis in the early universe can be dominated by fission cycling. Fission cycling occurs when neutrons are much more abundant than heavy nuclei and the neutron irradiation lasts a long time. In fission cycling a heavy nucleus absorbs neutrons and undergoes beta decays until it reaches $A \approx 260$, at which time it fissions. Binary fission produces two heavy nuclei, both of which can absorb neutrons and grow. Their fission produces four heavies, then eight, then 16, and so on. After N fission cycles the abundance of heavy nuclei has been increased by a factor of 2^N . A detailed discussion of fission cycling is given in the discussion of the long-time solution to the r -process by Seeger, Fowler, & Clayton (1965). The cycle time, the time needed for a single fission cycle, is a crucial parameter. For high neutron densities the cycle time is the sum of the beta-decay lifetimes along the nucleosynthesis path. The cycle time depends on the nucleosynthesis path because beta-decay lifetimes increase as the path approaches the valley of stability. Since the path moves away from the valley of stability as the external neutron density increases, the cycle time depends on the neutron density. In their calculations, Applegate et al. (1988) found that fission cycling was important and that many cycles could occur, but they could not calculate the actual number because they did not compute the nucleosynthesis path self-consistently with the changing neutron density. In this paper we compute the synthesis of heavy elements in neutron-rich environments fully self-consistently using a detailed reaction network. We find that the production of heavy elements is very sensitive to baryon density, and we trace roughly half of the density dependence to the increase of the cycle time with decreasing neutron density. A preliminary version of this work has already appeared (Thielemann et al. 1991).

A major difference between a phase transition in the early universe and one in the laboratory is that gravitation intro-

duces a dimensional parameter into the cosmological problem which is not present in the laboratory. This means that the natural scales of length and time in cosmology are not characteristic of pure particle physics but are determined by a combination of particle physics and gravity. For example, in the case of QCD, the critical temperature and energy density (excluding the photon and lepton contributions) at the phase transition are the same in the early universe as they are in the laboratory if the baryon density is low, as it should be in the central rapidity region of an ultrarelativistic heavy-ion collision. The lifetime of the quark-gluon plasma in such a collision is expected to be roughly 10^{-22} s, a characteristic strong interaction timescale for an object 10 fm in size. The duration of the cosmological phase transition is determined by the expansion rate of the universe at temperature T_c , which is roughly $\Delta t \sim (G\rho)^{-1/2} \sim 10^{-5}$ s, where $\rho = E/c^2$ is the mass density at the phase transition. The characteristic length scale of the density inhomogeneities is determined by the horizon distance $ct_c \sim 3$ km, where t_c is the age of the universe at the phase transition and the amount of supercooling $\Delta T/T_c$ in the transition. Since the rate of nucleation of the low-temperature phase is zero at the critical temperature, the universe will continue to expand in the quark-gluon plasma state for a time $\Delta t_N \sim t_c(\Delta T/T_c)$ before rapid nucleation occurs. Once nucleation occurs, the release of latent heat drives shocks into the quark-gluon plasma, heating it back toward T_c and shutting off further nucleation. The length scale L of the inhomogeneities is the distance between nucleation sites when the shocks from different sites overlap. If Δt_s is the time needed for the shocks to overlap, the length scale is $L \sim c\Delta t_s$. Detailed calculations (Hogan 1983; DeGrand & Kajantie 1984) show that to a very rough approximation $\Delta t_N \sim \Delta t_s$, which gives $L/ct_c \sim \Delta T/T_c$. Thus, supercooling of a few percent can produce structure on scales of hundreds of meters. This whole scenario depends on a first-order phase transition which leads to the release of latent heat. Calculations to determine the order of the QCD transition (Gottlieb et al. 1987; Fukugita, Okawa, & Ukawa 1989; Kogut & Sinclair 1988; Brown et al. 1990; Vaccarino 1991; Fukugita & Hogan 1991) obtained varying results. However, calculations with realistic quark masses are not conclusive yet, as they still require quite a number of approximations (for more details see Bonometto & Pantano 1993).

The expansion of the universe has been adiabatic from the QCD transition at a temperature of 10^{12} K (100 MeV) to roughly 1 K now. Adiabatic cooling of radiation by a factor of 10^{12} requires expanding all lengths by the same factor, so the 10^4 cm characteristic length of the inhomogeneities has expanded to 10^{16} cm now. This is about 1000 times the distance from the Earth to the Sun and about 1% the distance to the nearest star, tiny by astronomical standards. The baryon mass within the horizon at the QCD phase transition is roughly 10^{22} g, which is the mass of a large asteroid. These inhomogeneities have nothing to do with the formation of galaxies or other large-scale structure in the universe. The neutron- and proton-rich environments are completely mixed by the time the first stars in the Galaxy form. We can infer the existence of the neutron-rich environments, if they existed, because the heavy elements they synthesized will survive today as a cosmological minimum abundance of heavy elements. Also, the abundance pattern will be characteristic for fission cycling, which is not the case for stellar *r*- and *s*-processes.

We note that linear expansion offers a possible comparison of the extrapolations required in detecting a quark-gluon

plasma in the early universe and in heavy-ion collisions. In the laboratory, matter must expand from nuclear dimensions of roughly 10 fm to detector dimensions of roughly 10 m, a linear expansion by a factor of 10^{15} . The quark-gluon plasma in the early universe is three orders of magnitude closer than the quark-gluon plasma in the laboratory. We do note, however, that the final-state interactions are more complicated (and interesting) in cosmology than in heavy-ion collisions.

In the investigations carried out in this paper we are not concerned with how the inhomogeneities were generated, but we want to focus on the effect of such inhomogeneities on primordial nucleosynthesis. In this paper we undertake a detailed study of one of the proposed signatures of inhomogeneous nucleosynthesis—the production of very heavy elements by neutron capture—in several scenarios with different baryon-to-photon ratios η and with varying length scales L . Earlier attempts treated nuclei as heavy as Si (Kajino et al. 1990). Here we consider for the first time nuclei as heavy as $Z = 100$. A full charged-particle network from neutrons and protons up to Kr is coupled with a neutron capture *r*-process network up to $Z = 100$. Nuclei extend from stability to the neutron drip line. We find that under optimum conditions some significant neutron capture nucleosynthesis to very heavy nuclei is possible.

In § 2 we present the framework of our inhomogeneous big bang calculations, including the treatment of neutron back-diffusion. Section 3 describes the nuclear network employed. Section 4 focuses on the new reaction rates required for this undertaking, mostly charged particle and neutron capture reactions for nuclei between Li and Ne, where statistical model approaches do not work yet, because of low resonance densities. Section 5 contains the major set of calculations on an extended grid of baryon-to-photon ratios η and separation length L between high-density zones. The latter control the efficiency of neutron back-diffusion. The general reaction flow pattern as a function of η and L is analyzed in detail for the low-density neutron-rich zones, the only site where *very heavy* element production can be expected. Recent calculations by Jedamzik et al. (1993) also analyzed hydrodynamic effects (including shock waves not considered so far) and conditions where very high baryon densities allow for the production of heavy elements via the triple-alpha reaction. Such zones would not produce elements beyond Fe, which are only accessible via neutron capture. Section 6 discusses our results in view of observational and theoretical constraints on the parameter space and thus comes to conclusions for the results under realistic conditions.

2. INHOMOGENEOUS BIG BANG IN A TWO-ZONE MODEL

In the following we describe the methods used to calculate the initial conditions and the temperature and density evolution in high- and low-density regions during the expansion, and we present an analytical treatment of neutron diffusion.

2.1. Global Relations

The physical conditions during the expansion of the early universe are set by the Friedmann equations and the first law of thermodynamics,

$$\left(\frac{\dot{R}}{R}\right)^2 = H(t)^2 = \frac{8\pi G}{3c^2} \rho, \quad (1a)$$

and

$$\frac{d(\rho R^3)}{dt} + P \frac{dR^3}{dt} = 0, \quad (1b)$$

where ρ denotes the energy density. In the relativistic limit $kT \gg mc^2$, which is the case for the whole early radiation-dominated phase, we have $P = \rho/3$, and, therefore, equation (1b) leads to $\rho R^4 = \text{constant}$, and consequently equation (1a) to $\dot{R} \propto R^{-1}$. The solution is $R(t) \propto t^{1/2}$. On the other hand, $\rho \propto gT^4$ with $g = 3.3626$ in the radiation-dominated phase after weak decoupling, and equation (1a) gives a relation between $1/t^2$ and T^4 , with its precise form being (Börner 1988; Kolb & Turner 1990)

$$t = \left(\frac{3c^2}{16\pi G a} \right)^{1/2} g^{-1/2} \frac{1}{T^2} \quad \text{or} \quad T_9 = \frac{13.336}{t^{1/2}}. \quad (2)$$

With a global baryon-to-photon ratio $n_b/n_\gamma = \eta$ and the photon number density given by a Planck distribution $n_\gamma = 2.404/\pi^2(kT/\hbar c)^3$, one can express the baryon number density as a function of temperature:

$$n_b = 2.029 \times 10^{28} \eta T_9^3 \text{ cm}^{-3}$$

$$\text{or} \quad \rho_b = n_b m_u = 3.376 \times 10^4 \eta T_9^3 \text{ g cm}^{-3}, \quad (3)$$

when we neglect the small effects of binding energy or neutron-proton mass difference in comparison to the nuclear mass unit. This relation also yields the total neutron and proton densities, when introducing the neutron-to-proton ratio at the onset of nucleosynthesis after weak freeze-out and decay until $T = 0.1$ MeV, being $n/p = \frac{1}{2}$ with mass fractions $X_n = 0.125$ and $X_p = 0.875$ (Kolb & Turner 1990).

The standard big bang scenario assumes a homogeneous, isotropic expansion in a radiation-dominated universe without degenerate or exotic particles. The neutron-to-proton ratio, which constrains primordial nucleosynthesis, is determined by the conditions during weak decoupling at $T \approx 1$ MeV, when the electrons are no longer energetic enough to ensure an equilibrium by the reaction $p(e^-, \nu)n$, due to the neutron-proton mass difference of 1.3 MeV, and the positrons needed for the inverse reaction $n(e^+, \bar{\nu})p$ are no longer produced by pair creation. Primordial nucleosynthesis conditions are then determined by the particles remaining in thermal equilibrium, initial conditions at time t , and global adiabatic expansion. The initial conditions are set by neutrons, protons, electrons, and photons with densities n_n , n_p , n_e , and $n_\gamma = 2.404/\pi^2(kT/\hbar c)^3$. From charge neutrality it follows that $n_e = n_p$; n_p/n_n is given by the equilibrium ratio at weak freeze-out.

When the temperature declines during the expansion below 1 MeV, eventually the photodisintegration rate of ${}^2\text{H}$ (= deuterium, D) slows down. Then ${}^2\text{H}$ can be produced via neutron capture on protons. Nucleosynthesis proceeds when a substantial abundance of ${}^2\text{H}$ at $T_{D\gamma} \approx 0.1$ MeV $\approx 1.2 \times 10^9$ K enables further neutron, proton, and light nuclei capture to form ${}^3\text{H}$, ${}^3\text{He}$, ${}^4\text{He}$, and even heavier nuclei. However, the gaps existing among stable nuclei at mass numbers $A = 5$ and $A = 8$ inhibit the formation of nuclei beyond $A = 8$; therefore, the standard big bang can produce only ${}^2\text{H}$, ${}^3\text{He}$, ${}^4\text{He}$, and ${}^7\text{Li}$ in appreciable amounts. The strength of the standard big bang scenario is that only one free parameter must be specified, the baryon-to-photon ratio $\eta = n_b/n_\gamma$, to determine all of the primordial abundances, ranging over 10 orders of magnitude (see, e.g., Yang et al. 1984; Boesgaard & Steigman 1985; Kawano,

Schramm, & Steigman 1988; Olive et al. 1990; Walker et al. 1991). $\Omega_b = \rho_b/\rho_c$, $\rho_c = 3H_0^2/(8\pi G)$, and equation (3) for ρ_b yields a relation between Ω_b , the Hubble constant H_0 , and T :

$$\Omega_b h_{50}^2 = 1.54 \times 10^{-2} (T_9/2.78 \text{ K})^3 \eta_{10}, \quad (4)$$

using all quantities at the present time. The relation for the critical density ρ_c follows from the Friedmann equation for the (Hubble) expansion of the universe, $H(t)^2 = 8\pi G\rho/3 - k/R^2$ for a flat universe with $k = 0$ and therefore critical density ρ_c . $H_0 = h_{50} \times 50 \text{ km s}^{-1} \text{ Mpc}^{-1}$ and T_9 denote the Hubble constant and the present temperature of the microwave background.

The abundances of individual nuclei depend on η in the following way: A high (baryon) density during the nucleosynthesis phase, i.e., a large η , gives rise to a larger number of capture reactions on ${}^2\text{H}$ and ${}^3\text{He}$, and consequently leaves less ${}^2\text{H}$ and ${}^3\text{He}$ but increases the ${}^4\text{He}$ abundance. The behavior of the ${}^7\text{Li}$ abundance is more complex. At low densities ${}^7\text{Li}$ is produced via ${}^3\text{H}(\alpha, \gamma){}^7\text{Li}$, but is destroyed at higher densities by ${}^7\text{Li}(p, \alpha){}^4\text{He}$. However, increasing densities lead also to a larger production of ${}^7\text{Be}$ via ${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$, which is preserved during the nucleosynthesis period and subsequently decays to ${}^7\text{Li}$. This leads to a predicted minimum in the ${}^7\text{Li}/{}^1\text{H}$ ratio of about 10^{-10} , for $2 < \eta_{10} < 4$.

Primordial abundance information (see Boesgaard & Steigman 1985; for updates see Pagel 1987; Bania, Rood, & Wilson 1987; Spite & Spite 1986; Hobbs & Duncan 1987; Hobbs & Pilachowski 1988; Rebolo, Molaro, & Beckman 1988; Olive et al. 1990; Pagel 1991; Walker et al. 1991; Smith, Kawano, & Malaney 1993) results in the following limits: $({}^2\text{H}/{}^1\text{H}) \geq 1.8 \times 10^{-5}$, $({}^3\text{He}/{}^1\text{H}) \leq 1.8 \times 10^{-5}$, $({}^2\text{H} + {}^3\text{He}) \leq 9.9 \times 10^{-5}$, $({}^7\text{Li}/{}^1\text{H}) \leq 1.4 \times 10^{-10}$, and $0.22 \leq X_\alpha \leq 0.24$ (He mass fraction, often also called Y_p). Combining theoretical model predictions with this primordial abundance information, utilizing also the new neutron half-life of $\tau_{1/2} = 10.25 \pm 0.015$ minutes by Mampe et al. (1989), leads to the following conclusions: $2.8 \leq \eta_{10} \leq 4.0$ and $N_\nu \leq 3.3$. This can be translated to $\Omega_b h_{50}^2 = 0.05 \pm 0.01$. When a Hubble constant H_0 in the range 40–100 is used this is equivalent to a baryon density in the universe of $0.01 \leq \Omega_b \leq 0.10$ (see also the recent results by Songaila et al. 1994).

2.2. Relations for the Two-Zone Model

While equations (1)–(4) determine the conditions in the homogeneous standard big bang completely, they only apply globally in inhomogeneous scenarios. In the simplest of all cases, which was followed in our calculation of heavy elements, we assume a constant density in high- and low-density regions. This leads to the neutron and proton number densities n_n^h , n_n^l , n_p^h , and n_p^l in the high- and low-density regions. In each of the separated regions the n/p ratio is given by the global weak freeze-out values. The total baryon density follows equation (3), the density contrast between the two regions is $R = n_b^h/n_b^l = \rho_b^h/\rho_b^l$ (not to be confused with the scale factor in eq. [1]), and their respective volume fractions are f_v and $1 - f_v$. This determines the neutron and proton densities fully, because the mass fractions X_n (or X_p) are the same in each region. The baryon densities are related by $\rho_b = f_v \rho_b^h + (1 - f_v) \rho_b^l$, which leads with the density ratio R between high- and low-density region to

$$\frac{\rho_b^l}{\rho_b} = \frac{1}{f_v R + 1 - f_v} \quad \text{and} \quad \frac{\rho_b^h}{\rho_b} = \frac{R}{f_v R + 1 - f_v}. \quad (5)$$

The neutrons are assumed to diffuse out uniformly from these initial conditions. This will change the density contrast and the neutron density in both regions. The protons are, however, assumed to remain in place. When the superscripts 1 and 2 rather than h and l are used for this new situation, the following relations hold: $n_n^1 = n_n^2$ and $n_p^1 = n_p^h$, $n_p^2 = n_p^l$. That translates into $X_n^1 \rho_1 = X_n^2 \rho_2 = X_n \rho_b$ and $X_p^1 \rho_1 = X_p^h \rho_b$, $X_p^2 \rho_2 = X_p^l \rho_b$, and ρ_1 and ρ_2 can be expressed by the global quantities X_n , ρ_b and the parameters R and f_V :

$$\begin{aligned}\rho_1 &= X_n^1 \rho_1 + X_p^1 \rho_1 = X_n \rho_b + (1 - X_n) \rho_b^h, \\ \rho_2 &= X_n^2 \rho_2 + X_p^2 \rho_2 = X_n \rho_b + (1 - X_n) \rho_b^l.\end{aligned}$$

It is now easy to determine the ratios ρ_1/ρ_b and ρ_2/ρ_b :

$$\frac{\rho_1}{\rho_b} = X_n + \frac{(1 - X_n)R}{f_V R + 1 - f_V}, \quad \frac{\rho_2}{\rho_b} = X_n + \frac{(1 - X_n)}{f_V R + 1 - f_V}. \quad (6)$$

Equation (6) allows us to express the neutron and proton mass fractions in regions 1 and 2, respectively, as a function of the global mass fractions and the parameters R and f_V :

$$X_n^1 = X_n \frac{\rho_b}{\rho_1} = \frac{X_n}{X_n + (1 - X_n)R/(f_V R + 1 - f_V)}, \quad (7)$$

$$X_n^2 = X_n \frac{\rho_b}{\rho_2} = \frac{X_n}{X_n + (1 - X_n)/(f_V R + 1 - f_V)},$$

$$X_p^1 = X_p \frac{\rho_b^h}{\rho_1} = \frac{(1 - X_n)R/(f_V R + 1 - f_V)}{X_n + (1 - X_n)R/(f_V R + 1 - f_V)}, \quad (8)$$

$$X_p^2 = X_p \frac{\rho_b^l}{\rho_2} = \frac{(1 - X_n)/(f_V R + 1 - f_V)}{X_n + (1 - X_n)/(f_V R + 1 - f_V)}.$$

These relations had already been derived by Fuller et al. (1988), when one replaces the densities ρ in our formulation by the corresponding values for Ω_b . Now the temperature relation (eq. [2]), the density relations for ρ_b (eq. [3]), and ρ_1 and ρ_2 (eqs. [6]), as well as the determination of $X_n^{1,2}$ as a function of the global freeze-out value X_n and the values for η , f_V , and R in equations (7) and (8), lead to a uniquely defined initial-value problem. One can recognize that for the low-density region 2 all quantities depend only on the product $f_V R$ for large values of this product (f_V itself can only range between 0 and 1). The scenario described above is an oversimplification, not following the weak freeze-out in detail, assuming two regions with uniform densities and complete neutron diffusion before the onset of nucleosynthesis, while proton diffusion is treated as negligible (therefore a length scale L does not appear). In the following subsection we want to focus on an analytical description of the neutron (back-) diffusion into the proton-rich zones during nucleosynthesis (where the length scale of inhomogeneities will appear).

2.3. The Diffusion of Neutrons

Once produced, baryon density inhomogeneities begin to diffuse away. The diffusion is dominated by the particle with the longest mean free path, the neutron. As long as the weak interactions are in equilibrium, neutrons and protons diffuse together. Neutrons diffuse by diffusing. Protons diffuse by changing into neutrons, diffusing, and changing back. More precisely, the transport of baryon number is due entirely to the transport of neutrons, but as long as the weak interactions are fast enough to keep up with the expansion of the universe, the

local ratio of neutrons to protons is given by the Boltzmann factor, $\exp(-\Delta mc^2/kT)$. Neutron diffusion before weak decoupling erases small-scale inhomogeneities but does not produce variations in the local ratio of neutrons to protons.

The weak interactions fall out of equilibrium at the decoupling temperature $T_{\text{weak}} \simeq 1$ MeV when the universe is about 1 second old. After weak decoupling, protons stay protons and neutrons stay neutrons (the correction for free neutron decay is small). The mean free path of the proton is very short because of its electrical charge, so the proton distribution is effectively frozen at weak decoupling. The neutrons continue to diffuse, and now retain their identity as neutrons. Detailed calculations (Applegate et al. 1987; Applegate 1988) show that neutrons can diffuse to uniformity over very large comoving length scales by the time nucleosynthesis begins. This differential diffusion of neutrons and protons converts baryon density inhomogeneities into variations in the local neutron-to-proton ratio. If the amplitude of the initial inhomogeneities is large enough, some regions of the universe can undergo nucleosynthesis in environments in which neutrons locally outnumber protons. The possible production of heavy elements by successive neutron capture in these neutron-rich regions is the subject of this paper.

The character of neutron diffusion changes once nucleosynthesis begins. Once nucleosynthesis begins, ${}^4\text{He}$ is rapidly produced until one of the primary reactants, neutrons or protons, is exhausted. Neutrons are exhausted in a proton-rich environment. A neutron-rich region will exhaust its supply of protons, leaving it with a residual supply of neutrons. If neutron- and proton-rich environments coexist, the onset of nucleosynthesis will produce neutron density gradients which drive the diffusion of neutrons out of the neutron-rich regions and into the proton-rich ones. Once in a proton-rich environment, a neutron is rapidly captured by a proton and ultimately ends up in an alpha particle.

The three stages of neutron diffusion are shown in cartoon form in Figures 1a, 1b, and 1c. Figure 1a shows the distribution of protons (dotted line) and neutrons (solid line) around an underdense region with the weak interactions in equilibrium. The ratio of neutrons to protons is given by the same Boltzmann factor $\exp(-\Delta mc^2/kT)$ everywhere. The situation after weak decoupling but before nucleosynthesis is shown in Figure 1b. In this stage the neutrons have diffused to uniformity, while the proton distribution remains frozen at the shape it had at weak decoupling. Neutron diffusion during nucleosynthesis is illustrated in Figure 1c. The neutrons in the proton-rich region have all been consumed by protons, while there is a supply of neutrons in the neutron-rich region. The gradient of the neutron density drives neutron diffusion back into the proton-rich region. The sharp discontinuity of the neutron density gradient at the boundary is due to the fact that the neutron diffusion coefficient is much smaller in the proton-rich region than in the neutron-rich region (see below).

In the following we discuss the modifications to our reaction network that are required to treat neutron diffusion during nucleosynthesis. We find that a careful choice of the definition of the abundance by number, Y_i , is the only modification required for all of the equations in the network except the one describing the evolution of the neutron abundance. The loss of neutrons due to diffusion out of the region must be accounted for explicitly in the neutron equation. To do this, we refine the analytical treatment of diffusion during nucleosynthesis introduced by Applegate (1988) and Applegate et al. (1988).

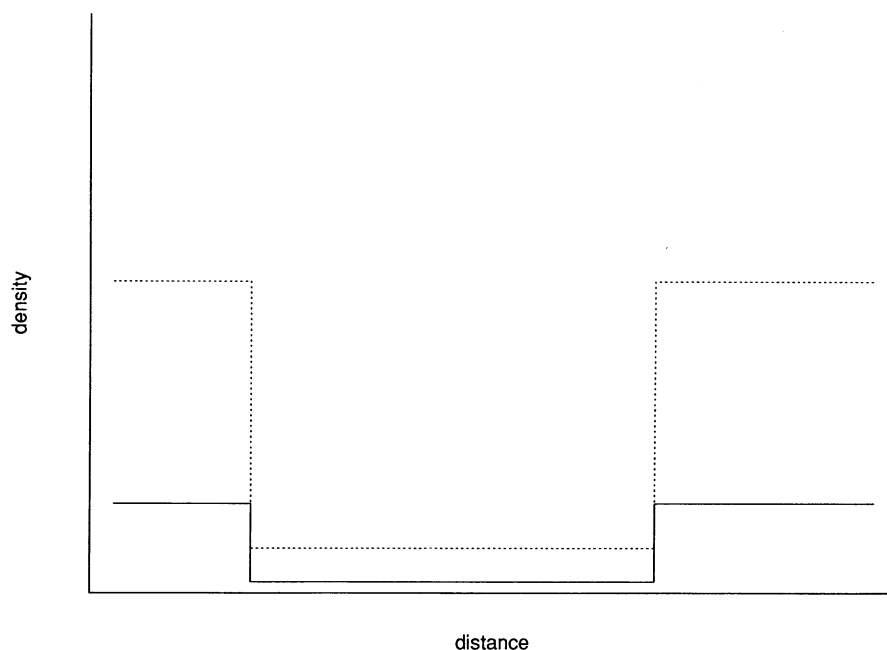


FIG. 1a

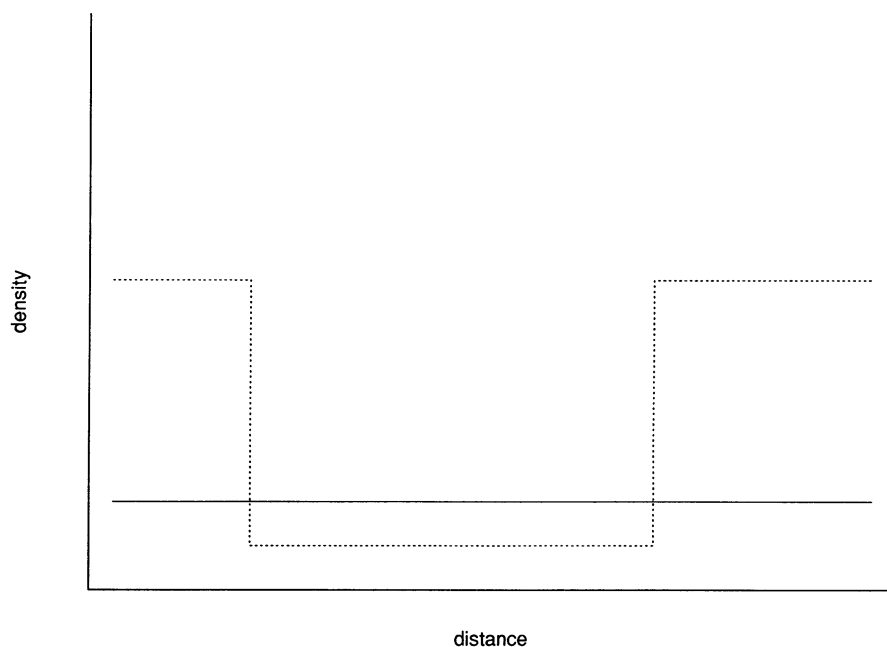


FIG. 1b

FIG. 1.—Time evolution of neutron diffusion (solid lines refer to neutron densities and dotted lines to proton densities). (a) Before the weak freeze-out, neutron and proton densities follow the global density pattern and n/p ratio. (b) After weak freeze-out and before the onset of nucleosynthesis, the neutrons diffuse to a uniform density, while the protons retain the original global density pattern, due to the short mean free path of protons. (c) After the onset of nucleosynthesis, neutrons are immediately consumed in the high-density regions with a small n/p ratio, and neutron back-diffusion from the low-density (high n/p) regions becomes the only source of fresh neutrons.

Consider the rate equations for all nuclear species other than neutrons. Let $N_k(t)$ be the number of nuclei of species k contained within a comoving volume $V(t)$, and let $N_B(t)$ be the number of baryons contained within V . The total baryon number is time-dependent because of the diffusion of neutrons out of the volume. A natural choice for the definition of the abundance by number for species k would be to set $Y_k(t) = N_k(t)/N_B(t)$. We find this a poor choice because this definition

requires that every equation in our network be modified for diffusion. The simple example of a radioactive decay will illustrate the problem. The rate of change of N_k due to radioactive decay is described by

$$\frac{dN_k}{dt} = -\lambda_k N_k. \quad (9)$$

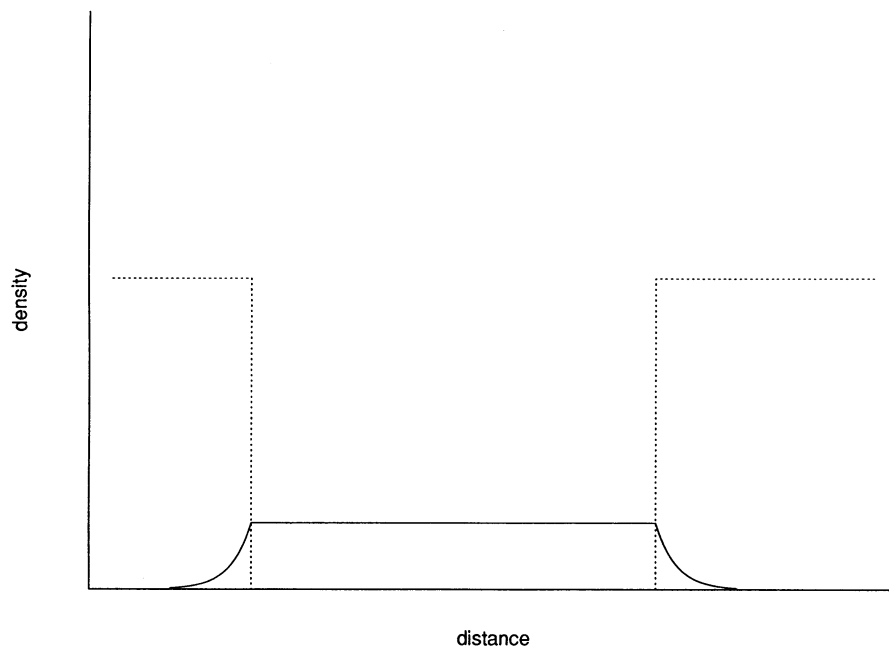


FIG. 1c

With the definition $N_k(t) = Y_k(t)N_B(t)$ this equation becomes

$$\frac{dY_k}{dt} = -\lambda_k Y_k - Y_k \frac{d \ln N_B}{dt}. \quad (10)$$

The second term on the right-hand side of equation (10) is due to the time dependence of the baryon number $N_B(t)$. The presence of this term causes us to seek a better generalization of our network equations.

We define the abundance of species k as

$$Y_k(t) = \frac{N_k(t)}{N_0}, \quad (11)$$

where $N_0 = N_B(t=0)$ is the number of baryons in the volume at the beginning of the calculation. Since N_0 is a constant, the objectionable term in equation (10) does not arise. With this definition, any one-body reaction, such as radioactive decay, is described by

$$\frac{dY_k}{dt} = -\lambda_k Y_k. \quad (12)$$

The rate of change of N_k due to particles of species k and i reacting to form something else in a two-body reaction is given by

$$\frac{dN_k}{dt} = -N_k \frac{N_i}{V(t)} \langle \sigma v \rangle_{ki}, \quad (13)$$

where $\langle \sigma v \rangle_{ki}$ denotes a thermal average of the σv appropriate to the reaction. With the abundance defined in equation (11), this becomes

$$\frac{dY_k}{dt} = -Y_k Y_i n_0 \langle \sigma v \rangle_{ki}, \quad (14)$$

where $n_0 = N_0/V(t)$ is the baryon density uncorrected for diffusion. This is exactly the same equation that describes the reaction in the absence of diffusion, just replacing $N_B(t)$ by N_0 .

With our definition of abundance, the equations describing one- and two-body reactions in the presence of diffusion are exactly the same as in the absence of diffusion. A straightforward calculation shows that the expression for three-body reactions is also unmodified.

In the absence of diffusion the conservation of baryon number implies that $\sum A_k Y_k = 1$, where A_k is the mass number of nuclear species k . In the presence of diffusion and with our definition of abundance, the conservation of baryon number becomes $\sum A_k Y_k = 1 - Y_n^{\text{diff}}$, where Y_n^{diff} is the abundance of neutrons which have diffused out of the neutron-rich region. If N_n^{diff} is the number of neutrons that have diffused out, Y_n^{diff} is defined to be $Y_n^{\text{diff}} = N_n^{\text{diff}}/N_0$. The abundance of lost neutrons can be obtained by integrating equation (16).

To derive the requisite modification to the rate equation for neutrons, we begin with the diffusion equation for neutrons in an expanding medium,

$$\frac{dn_n}{dt} + n_n \nabla \cdot \mathbf{v} = \nabla \cdot (D \nabla n_n), \quad (15)$$

where $n_n = N_n(t)/V(t)$ is the neutron density, D is the diffusion coefficient for neutrons, and $\mathbf{v} = H(t)\mathbf{r}$ is the velocity field of cosmological expansion. The comoving volume $V(t)$ and Hubble constant $H(t)$ are related to $R(t)$ and $\dot{R}(t)$ via $V \propto R^3$ and $H = \dot{R}/R$ (see eq. [1a]). The neutron abundance is $Y_n = n_n/n_0$, with the same $n_0 = N_0/V(t)$ as defined above. The time derivative of the neutron density is $\dot{n}_n = n_0 \dot{Y}_n + Y_n \dot{n}_0$. The time dependence of the baryon density n_0 is due entirely to expansion; thus $\dot{n}_0 + n_0 \nabla \cdot \mathbf{v} = 0$ and $Y_n \dot{n}_0 + n_n \nabla \cdot \mathbf{v} = 0$. The remaining terms in equation (15) give the additional term required to account for diffusion:

$$\left(\frac{dY_n}{dt} \right)_{\text{diffusion}} = \frac{1}{n_0} \nabla \cdot (D \nabla n_n). \quad (16)$$

The total rate of change of the neutron abundance is obtained by adding the diffusion term to the rate equation for neutrons in the reaction network.

We evaluate the diffusion term for neutrons using the one-dimensional treatment of Applegate (1988) and Applegate et al. (1988). We let the region from $x = 0$ to $x = L$ be neutron-rich (introduced as region 2 in the previous section), and we let the region from $x = L$ to $x = \infty$ be proton-rich (region 1). We assume symmetry about the origin. We assume that at the beginning of the calculation the baryon density is constant in each of these regions and discontinuous at $x = L$. The rate equation for neutrons in the neutron-rich region is

$$\dot{Y}_n = \frac{\partial}{\partial x} \left(D_2 \frac{\partial Y_n}{\partial x} \right) + \Gamma_2 - \lambda_2 Y_n, \quad (17)$$

where D_2 is the diffusion coefficient for neutrons in the neutron-rich region, Γ_2 is the rate at which reactions produce neutrons, and λ_2 is the rate at which neutrons are consumed by reactions. If the neutron-rich region is not too large (in a sense to be made precise below), the diffusion term in equation (17) will be dominated by the lowest mode of the diffusion equation. The lowest spatial mode is $Y_n(x) = Y_n(0) \cos(\alpha x)$, with α to be determined by the boundary conditions. With this, the neutron rate equation becomes

$$\dot{Y}_n = \Gamma_2 - (D_2 \alpha^2 + \lambda_2) Y_n; \quad (18)$$

the diffusion term enters the rate equation in exactly the same way as all of the other neutron loss terms. The effect of the diffusion of neutrons out of the neutron-rich region is to subtract a diffusive loss term $\dot{Y}_n^{\text{diff}} = -\kappa Y_n$, with $\kappa = D_2 \alpha^2$, from the rate equation for neutrons in the neutron-rich zone. The value of the diffusive loss term is determined by the conditions at the boundary between the neutron- and proton-rich zones.

The rate equation for neutrons in the proton-rich region is

$$\dot{Y}_n = \frac{\partial}{\partial x} \left(D_1 \frac{\partial Y_n}{\partial x} \right) + \Gamma_1 - \lambda_1 Y_n, \quad (19)$$

where D_1 , Γ_1 , and λ_1 are the neutron diffusion coefficient, production rate, and absorption rate in the proton-rich region. There are no reactions which liberate neutrons in significant numbers in the proton-rich zone, so we set $\Gamma_1 = 0$. The neutron abundance in region 1 is a balance between diffusion in from the neutron-rich region and radiative capture by protons to form deuterium. Once captured by a proton, a neutron ultimately finds its way into an alpha particle. Radiative capture by protons is fast, typically of order $\lambda_1 \sim 1 \text{ s}^{-1}$. The neutron profile in region 1 changes much more slowly, requiring times of the order of the Hubble time, 300–1000 s, to change significantly. Physically, this means that the neutron profile is in a steady state; neutron capture by protons balances neutron addition by diffusion. Mathematically, this means that the time derivative on the left-hand side of equation (19) is much smaller than the diffusion or capture terms on the right-hand side. The diffusion term and the capture term on the right-hand side of equation (19) cancel each other almost exactly. Thus, the spatial dependence of the neutron density in region 1 is given by

$$D_1 \frac{\partial^2 Y_n}{\partial x^2} - \lambda_1 Y_n = 0, \quad (20)$$

which gives

$$Y_n(x) = Y_n(L) e^{-\beta(x-L)}, \quad (21)$$

with $\beta^2 = \lambda_1/D_1$.

The boundary conditions at $x = L$ are that the neutron density n_n and the neutron flux $-D \partial n_n / \partial x$ must be continuous. The solutions of the diffusion equation in regions 1 and 2 are

$$n_1(x) = N_1 e^{-\beta(x-L)}$$

and

$$n_2(x) = N_2 \cos(\alpha x),$$

where $n_1(x)$ and $n_2(x)$ are the neutron densities in regions 1 and 2, and N_1 and N_2 are normalization coefficients. The continuity of the neutron density gives $N_2 \cos(\alpha L) = N_1$, and the continuity of the neutron flux gives $\alpha D_2 N_2 \sin(\alpha L) = \beta D_1 N_1$. These may be combined with the definition of β to give

$$D_2 \alpha \tan(\alpha L) = (D_1 \lambda_1)^{1/2}. \quad (22)$$

We consider only neutron-rich regions small enough for $\alpha L < 1$. Free neutron decay dominates diffusion for larger regions, so diffusion can be neglected. In addition, our approximations are not valid if $\alpha L > 1$. If we set $\tan x = x$ in equation (22) and use the expression for the diffusive loss rate κ derived above, we obtain

$$\kappa = D_2 \alpha^2 = \frac{(\lambda_1 D_1)^{1/2}}{L}, \quad (23)$$

This result was derived in slightly more generality by Applegate et al. (1988) and Applegate (1988). With this, the rate equation for neutrons in the neutron-rich zone is

$$\dot{Y}_n = \Gamma_2 - (\kappa + \lambda_2) Y_n, \quad (24)$$

with the diffusive loss rate κ given by equation (23).

The neutron capture rate in the proton-rich zone is $\lambda_1 = n_p \langle \sigma_{\text{abs}} v \rangle$, where σ_{abs} is the radiative capture cross section and n_p is the density of protons. The $\langle \sigma v \rangle$ for this reaction is (Fowler, Caughlan, & Zimmerman 1967)

$$\langle \sigma_{\text{abs}} v \rangle = 7.30 \times 10^{-20} (1 - 0.861 T_9^{1/2} + 0.429 T_9) \text{ cm}^3 \text{ s}^{-1}. \quad (25)$$

We approximate the neutron diffusion coefficient as $D_1 = v_T / 3 n_p \sigma_{\text{scatt}}$, where $v_T = 5 \times 10^8 T_9^{1/2} \text{ cm s}^{-1}$ is the velocity of a thermal neutron and σ_{scatt} is the cross section for neutron-proton elastic scattering. At the low energies we consider, this cross section may be evaluated using the effective range expression (Preston & Bhaduri 1975)

$$\sigma_{\text{scatt}} = \frac{\pi a_s^2}{(a_s k)^2 + (1 - r_s a_s k^2/2)^2} + \frac{3\pi a_t^2}{(a_t k)^2 + (1 - r_t a_t k^2/2)^2}, \quad (26)$$

where $a_s = -23.71 \text{ fm}$ and $a_t = 5.432 \text{ fm}$ are respectively the singlet and triplet scattering lengths, $r_s = 2.73 \text{ fm}$ and $r_t = 1.729 \text{ fm}$ are the singlet and triplet effective ranges, and $k^2 = 3k_B T / \hbar^2 \mu = 3.1 \times 10^{-3} T_9 \text{ fm}^{-2}$, where μ is the reduced mass of the neutron-proton system. The product $\lambda_1 D_1$ is

$$\lambda_1 D_1 = \frac{v_T \langle \sigma_{\text{abs}} v \rangle}{3 \sigma_{\text{scatt}}}, \quad (27)$$

independent of proton density. The diffusive loss rate κ does not depend on the density of protons in the proton-rich region.

The length L depends on the comoving length scale of the inhomogeneities. The entropy during the expansion $[\propto g T^3 V]$, where $g = g_{\text{bos}} + (7/8) g_{\text{ferm}}$, the statistical weight of all

(relativistic) species, which dominate pressure, entropy and energy density] is constant. With $V \propto L^3$, we also have $g^{1/3} L k T = \text{constant}$, or $L = L_0 (g_0/g)^{1/3} (k T_0)/(k T)$, where the subscript zero corresponds to the initial values at the QCD phase transition (≈ 100 MeV). Applegate et al. (1988) introduced the term “comoving length scale,” $(d/a) = L_0 (g_0/g)^{1/3} k T_0$. At the phase transition g_0 is determined by the relativistic particle families γ , π , μ , e , and ν with $g_0 = 138/8$. At temperatures close to 1 MeV only photons, electrons, positrons, and the three neutrino families contribute; thus $g = 86/8$, or $(g_0/g)^{1/3} = 1.17$. For temperatures below 1 MeV after weak decoupling and annihilation of $e^+ e^-$ pairs, the $e^+ e^-$ entropies are transferred to photons and the photon (and matter) temperature is higher than the (neutrino) temperature by $(11/4)^{1/3}$ (Kolb & Turner 1990). Thus we have two relations for the length scale L_0 at the phase transition and L during nucleosynthesis:

$$L_0 = \left(\frac{g}{g_0}\right)^{1/3} \frac{1}{k T_0} \left(\frac{d}{a}\right) = \frac{1}{1.17 k T_0} \left(\frac{d}{a}\right)$$

$$L = \frac{1}{k T_\nu} \left(\frac{d}{a}\right) = \frac{(11/4)^{1/3}}{k T_\nu} \left(\frac{d}{a}\right) = \frac{16.3 \text{ MeV}}{T_9} \left(\frac{d}{a}\right)_{\text{cm MeV}}. \quad (28)$$

In our calculations we consider d/a in the range $10^{5.5} - 10^{7.5}$ cm MeV (see also Applegate et al. 1988). This corresponds to an $L_0(100 \text{ MeV})$ at the QCD phase transition between 27 and 2700 m. Neutron-rich zones smaller than $d/a \sim 10^5$ cm MeV will lose their neutrons so fast that no heavy-element nucleosynthesis will occur, while neutrons cannot diffuse to uniformity over lengths of much more than 10^7 cm MeV. These large regions will affect nucleosynthesis, but our treatment of neutron diffusion is not applicable.

The neutron diffusive loss rate κ can be obtained by combining equations (23)–(28). The temperature dependence of κ implicit in $\langle \sigma_{\text{abs}} v \rangle$ and σ_{scatt} , though complicated, is fairly weak. This temperature dependence can be parameterized and a simple expression for κ derived. In the temperature range relevant to primordial nucleosynthesis, $0.2 < T_9 < 1$, κ is given by

$$\kappa = \frac{4.2 \times 10^4}{(d/a)_{\text{cm MeV}}} T_9^{5/4} (1 + 0.716 T_9)^{1/2} \text{ s}^{-1} \quad (29)$$

to an accuracy of about 1%.

The analytical treatment of neutron diffusion described above is comparable in accuracy to high-resolution grids which treat the diffusion numerically (e.g., Kurki-Suonio et al. 1990) in order to measure the total loss of neutrons out of the neutron-rich zones. It only depends on the comoving length scale of inhomogeneities (d/a). Small separation lengths between high-density zones make the neutron leakage out of the small low-density zones most effective. Large separation lengths make the neutron leakage negligible. As we are only considering heavy-element production in this paper, we will not have to deal with either proton-rich zones or the interface.

3. THE NUCLEAR NETWORK

3.1. The Charged Particle Network

Our reaction network consisted of two parts, one part for light and intermediate nuclei and the second part an r -process code. For light and intermediate nuclei from neutrons and protons to krypton ($Z = 36$), from stability to the neutron drip line, we made use of a general nuclear network (of 655 nuclei) which includes neutron, charged particle, and photon-induced

reactions as well as weak reactions. The nuclear abundances as defined in § 2.3 (eq. [11]) are given by $Y_i = N_i/N_0$, the number of nuclei of species i in a given volume divided by the total number of baryons initially in this volume, before (back) diffusion of neutrons sets in. This can also be written as n_i/n_0 , where n_0 is the baryon number density uncorrected for diffusion. The regular expression for $Y_i = n_i/(\rho N_A) = n_i/n_b$ differs from this definition. Correspondingly, we have to replace $n_b = \rho N_A$ by $n_0 = \rho_0 N_A$ in the system of differential equations generally used in predicting the change of abundances. For a nucleus with atomic weight A_i , $A_i Y_i$ represents then only the mass fraction of this nucleus with respect to the baryonic mass before diffusion set in, therefore $\sum A_i Y_i = 1$ is only fulfilled initially. In terms of nuclear abundances Y_i , the reaction network is described by the following set of differential equations:

$$\dot{Y}_i = -\delta_{in} \kappa Y_n + \sum_j N_j^i \lambda_j Y_j + \sum_{j,k} N_{j,k}^i \rho_0 N_A \langle j, k \rangle Y_j Y_k$$

$$+ \sum_{j,k,l} N_{j,k,l}^i \rho_0^2 N_A^2 \langle j, k, l \rangle Y_j Y_k Y_l. \quad (30)$$

The density ρ_0 in equation (30) can be determined from equations (3) and (6), i.e., for the neutron-rich zone $\rho_0 = \rho_2$. This is the case because equation (6) was derived without taking into account diffusion and thus gives the uncorrected value. The right-hand side of equation (30) contains (1) the neutron diffusion term as defined in equations (23), (24), and (29); (2) decays, photodisintegrations, and electron and positron captures; (3) two-particle reactions; and (4) three-particle reactions like the triple-alpha process, which can be interpreted as successive captures with an intermediate unstable target (see, e.g., Nomoto, Thielemann, & Miyaji 1985). The individual N^i are given by $N_{j(k,l)}^i = N_i/N_{j(k,l)}$. The N^i can be positive or negative numbers and specify how many particles of species i are created or destroyed in a reaction. The factorials in the denominator count the number of identical particles among the reactants and avoid double counting of the number of reactions (for example, in the $^{12}\text{C} + ^{12}\text{C}$ or the triple-alpha reaction; for details see Fowler et al. 1967). This set of stiff differential equations is solved with a fully implicit treatment (see, e.g., Press et al. 1986, § 15.6), $\Delta Y_i/\Delta t = f_i(Y_i(t + \Delta t))$, where all quantities on the right-hand side are evaluated at time $t + \Delta t$. This results in a set of nonlinear equations for the new abundances $Y_i(t + \Delta t)$, which can be solved using a multidimensional Newton-Raphson iteration procedure.

3.2. The r -Process Network

The second part is an r -process code that determines the abundances of heavy nuclei. This network extends up to $Z = 114$ and contains all nuclei from the so-called valley of beta stability to the neutron drip line (see also Cowan, Cameron, & Truran 1983). The neutron capture rates were calculated with statistical model methods, and the beta-decay rates were taken from Klapdor, Metzinger & Oda (1984), where experimental values were not available (see also Cowan, Thielemann, & Truran 1991).

The numerical methods employed in the solution of the r -process rate equations involve the straightforward application of implicit differencing techniques. Consider the following representative segment of the nuclear reaction network:

$$\begin{array}{ccccc} (Z+1, A-2) & (Z+1, A-1) & (Z+1, A) & & \\ & (Z, A-1) & (Z, A) & (Z, A+1) & \\ & & (Z-1, A) & (Z-1, A+1) & (Z-1, A+2) \end{array}$$

We include all possible neutron capture and photodisintegration reactions, as well as beta decays leading to the emission of zero, one, two, or three delayed neutrons. The rate of change of the abundance of nucleus $Y(Z, A) = n(Z, A)/(\rho_0 N_A)$ is then given by

$$\begin{aligned} \dot{Y}(Z, A) = & n_n Y(Z, A-1) \sigma_{A-1} + Y(Z, A+1) \lambda_{A+1} \\ & - Y(Z, A) (n_n \sigma_A + \lambda_A + \lambda_{\beta 0}^A + \lambda_{\beta n}^A + \lambda_{\beta 2n}^A + \lambda_{\beta 3n}^A) \\ & + Y(Z-1, A) \lambda_{\beta}^{Z-1, A} + Y(Z-1, A+1) \lambda_{\beta n}^{Z-1, A+1} \\ & + Y(Z-1, A+2) \lambda_{\beta 2n}^{Z-1, A+2} \\ & + Y(Z-1, A+3) \lambda_{\beta 3n}^{Z-1, A+3}, \end{aligned} \quad (31)$$

where $n_n = Y_n n_0 = Y_n \rho_0 N_A$ is the neutron number density; σ_{A-1} is the thermally averaged (n, γ) reaction rate $\langle \sigma v \rangle$ of nucleus $(Z, A-1)$; λ_{A+1} is the photodisintegration rate (γ, n) for nucleus $(Z, A+1)$; and $\lambda_{\beta 0}^A, \lambda_{\beta n}^A, \lambda_{\beta 2n}^A$, and $\lambda_{\beta 3n}^A$ are the rates of beta decay of nucleus (Z, A) followed by the emission of zero to three neutrons.

In a fully implicit treatment, the stiff differential equations in equation (31) can be solved as discussed in § 3.1 and would result in a set of nonlinear equations for the new abundances $Y(Z, A, t + \Delta t)$. If we assume that n_n is constant (over a time step Δt), equation (31) leads to a set of linear equations for the ΔY 's, which can be solved with methods for tridiagonal matrices in case a reaction flow proceeds only from small Z 's to large Z 's (see Cowan et al. 1991 for details). This is essential and allows the advantages associated with the use of implicit techniques, even for a full r -process network containing 6033 nuclei.

For the calculations in this paper we also introduced (beta-delayed) fission of heavy nuclei, as calculated by Thielemann, Metzinger, & Klapdor (1983) with the Howard & Möller (1980) fission barriers and masses. Such a choice (although not perfect) is presently the most realistic and consistent treatment available (see Cowan et al. 1991). In this case nuclear fission cycles material from large Z 's back to smaller Z 's and a fission term $\lambda_{\beta f}(Z, A)Y(Z, A)$ has to be subtracted in equation (31). We lack the knowledge of fission yields for very neutron-rich nuclei, and therefore we have assumed symmetric fission. We do, however, also think that the assumption of symmetric fission is actually very accurate. Asymmetric ground-state fission is essentially caused by shell corrections to nuclear binding energies. It is known from experiments that the fission spectrum becomes symmetric for high excitation energies, when the excitation energy is of the order of the shell corrections to the nuclear binding. In an r -process we do not have ground-state fission but rather beta-delayed fission with typical beta-decay Q -values of 13 MeV. The largest possible shell effects are of the order of 16 MeV, i.e., we expect almost no remaining shell effects and thus symmetric fission.

Even if this would be wrong, it would cause no effect on the amount of fission cycling and the total amount of heavy elements produced. This is due to the fact that the total amount of neutrons, captured until a fissioning nucleus is produced from the products of the last fission event, is the same, whether one treats a distribution over A or takes $2A/2$. The only possible effect could be that nuclei with A smaller than $A/2$ do not appear in the abundance step between pure seed nuclei and nuclei enhanced by fission cycling. Thus, also a production term $\lambda_{\beta f}(Z_f, A_f)Y(Z_f, A_f)$ with $Z_f \approx 2Z$ and $A_f \approx 2A$ has to

be added. This cannot be treated implicitly within the method described above. Therefore, that part is implemented in an explicit way, limiting time steps in the r -process network to half-lives of beta-delayed fission of appropriate nuclei.

3.3. Network Coupling

These two networks are coupled together in such a way that they run simultaneously at each time step, and the number of neutrons produced and captured is transmitted back and forth between them. The neutron abundance Y_n is a variable in the charged particle network where the dominant abundances are retained which affect the neutrons. Then this neutron abundance is used to obtain the neutron number density $n_n = \rho_0 N_A Y_n$ in the r -process network and is assumed to be constant over the (same) time step. The flux between the two networks is determined by treating the Kr isotopic chain as a part of both networks. In each time step neutron captures and beta decays will lead to a (possibly artificially high) buildup of Kr in the charged particle network, due to the inhibition of beta decays of Kr isotopes and neutron captures by the most neutron-rich Kr isotope. The Kr abundances resulting from this application of the charged particle network are fed into the r -process code and given the chance to follow the correct path of neutron captures and beta decays for that time step, thus forming heavier nuclei. The next time step is started in the charged particle network with these Kr isotopic abundances from the r -process code. The neutron abundance change during the previous time step, due to nuclei beyond Kr, is given by the increase of the total mass fraction in the r -process network. It thus can be written as

$$\Delta Y_{n,r} = - \sum_{Z,A,r} A \Delta Y(Z, A), \quad (32)$$

where the same symbols are used as in equation (31). This is used as a correction to the neutron abundance in the charged particle network to ensure an accurate accounting of the number of neutrons produced and absorbed and to ensure mass conservation. The total abundances of all nuclei in both networks are initially normalized to $\sum_i A_i Y_i = 1$. This mass is, however, not conserved, due to the diffusion of neutrons (see § 2.3).

There exists one source of error in this treatment. In the case of small photodisintegration rates when only neutron captures are important, the Kr isotopes are exposed to neutron capture twice in one time step, once in the charged particle and once in the r -process network. When one is close to an $(n, \gamma) - (\gamma, n)$ equilibrium, photodisintegrations stabilize the abundances in each isotopic chain (i.e., also for Kr) and the position of the abundance peak remains fixed. Thus, any additional neutron capture is canceled by an additional photodisintegration and no error is introduced. Also, the error mentioned above is small with respect to the total process. Only small local disturbances, if any, are expected.

4. REACTION RATES AND THEIR DETERMINATION

The general basis for the individual rates in equations (30) and (31), $\lambda_j, N_A \langle j, k \rangle$, and $N_A^2 \langle j, k, l \rangle$ is formed by the following sources. Beta-decay half-lives, if not known experimentally, come from Klapdor et al. (1984); electron and positron captures from Fuller, Fowler, & Newman (1982, 1985); experimental nuclear rates for light nuclei from the most recent compilation by Caughlan & Fowler (1988); experimental neutron capture cross sections from Bao & Käppeler (1987);

and rates for unstable light nuclei are given by Malaney & Fowler (1988, 1989), Fowler (1993), Wiescher & Görres (1988), Wiescher et al. (1986, 1987, 1989a), and Wiescher, Görres, & Thielemann (1988, 1990). For the vast number of medium and heavy nuclei which exhibit a high density of excited states at capture energies, Hauser-Feshbach (statistical model) calculations are applicable, e.g., Thielemann, Arnould, & Truran (1987). For a detailed discussion of the methods involved and neutron capture cross sections for heavy unstable nuclei see also § 3.4 and the appendix in Cowan et al. (1991).

An overview over reactions, important in the standard big bang, is given in Yang et al. (1984) and Deliyannis et al. (1989). In an inhomogeneous big bang the breakout to heavier nuclei has to be considered. In addition, new reaction links, not considered previously, do become important. Neutron-rich light unstable nuclei from Li to Ne form an area of the nuclear chart, previously not investigated for thermonuclear reaction rates because no practical application was recognized. With the overwhelming abundance of neutrons in the low-density neutron-rich regions it is, however, quite feasible that neutron captures on unstable nuclei can bypass the relatively slow beta decays in this mass region. For this reason, we have investigated neutron capture reactions on Li, Be, B, C, N, O, F, and Ne isotopes, from stability to the neutron drip line.

The barriers that prevent the synthesis of heavy elements in a proton-rich environment, such as in standard big bang nucleosynthesis, do not apply in a neutron-rich environment. One of the surprises in the first calculations of nucleosynthesis under neutron-rich conditions was the large amount of ^{14}C produced (Applegate et al. 1987; Alcock et al. 1987; Malaney & Fowler 1987). Reactions starting with neutron captures on protons, $^1\text{H}(n, \gamma)^2\text{H}(n, \gamma)^3\text{H}(d, n)^4\text{He}(t, \gamma)^7\text{Li}$ led to the production of ^7Li , and the sequence $^7\text{Li}(n, \gamma)^8\text{Li}(\alpha, n)^{11}\text{B}(n, \gamma)^{12}\text{B}(\beta^-)^{12}\text{C}(n, \gamma)^{13}\text{C}(n, \gamma)^{14}\text{C}$ produces carbon. An alternate branching was $^7\text{Li}(\alpha, \gamma)^{11}\text{B}$. Additional alternative reactions such as $^7\text{Li}(t, n)^9\text{Be}(t, n)^{11}\text{B}$, $^8\text{Li}(n, \gamma)^9\text{Li}(\beta^-)^9\text{Be}$, $^8\text{Li}(d, p)^9\text{Li}$, $^8\text{Li}(d, n)^9\text{Be}$, and $^8\text{Li}(d, t)^7\text{Li}$ might also become important (Boyd & Kajino 1989; Kajino & Boyd 1990; Brune et al. 1991). If the neutron-rich nuclei ^9Li , ^{10}Be , and ^{13}B are produced, further (α, n) reactions can become important. We have investigated these rates with statistical model methods. At three positions (^7Li , ^9Be , and ^{11}B), proton-induced reactions would prevent the buildup of heavier nuclei in a standard big bang scenario and lead to the destruction of heavy nuclei instead via $^7\text{Li}(p, \alpha)^4\text{He}$, $^9\text{Be}(p, \alpha)^6\text{Li}$, or $^{11}\text{B}(p, 2\alpha)^4\text{He}$. Once ^{14}C has been produced, pathways to rich nuclei in neutron-rich environments exist (Applegate et al. 1988; Applegate 1988): e.g., $^{14}\text{C}(\alpha, \gamma)^{18}\text{O}(n, \gamma)^{19}\text{O}(\beta^-)^{19}\text{F}(n, \gamma)^{20}\text{F}(\beta^-)^{20}\text{Ne}(n, \gamma)^{21}\text{Ne}(n, \gamma)^{22}\text{Ne}$, etc. Once past the oxygen isotopes, the reactions are dominated by neutron captures and beta decays. There are considerable associated uncertainties, because many of these reactions involve unstable nuclei, and also most of the reactions on stable targets in this region of the nuclear chart are not well determined at present (Malaney & Fowler 1989; Fowler 1993).

In the following we want first to review the apparently major breakout reaction $^8\text{Li}(\alpha, n)^{11}\text{B}$ and other reactions between $Z = 3$ and $Z = 10$; we will then present the results from our neutron capture studies of nuclei from Li to Ne. Here we utilized all experimentally available information about resonances and bound states to determine direct capture and resonance capture neutron cross sections for nuclei in the range Li–F, where reaction rates were not available yet.

4.1. $^8\text{Li}(\alpha, n)^{11}\text{B}$ and Other Breakout Reactions

Because of the great interest and the experimental difficulties in measuring reactions involving the short-lived nucleus ^8Li ($\tau_{1/2} = 0.84$ s; Ajzenberg-Selove 1988), many different approaches have been taken to determine the $^8\text{Li}(\alpha, n)^{11}\text{B}$ cross section at thermonuclear energies. The first measurement (Paradellis et al. 1990) via the reverse reaction $^{11}\text{B}_{\text{gs}}(n, \alpha)^8\text{Li}$ showed the existence of a resonance in the energy region of interest, but could only give the contribution of the $^8\text{Li}(\alpha, n_0)$ reaction, proceeding to the ground state of ^{11}B . Kubono et al. (1991) analyzed the decay properties of the resonance state and found comparable contributions to the ground state and excited states of ^{11}B . A recent measurement (Boyd et al. 1992) tried to determine the total rate by directly measuring the forward reaction $^8\text{Li}(\alpha, n)^{11}\text{B}^*$. The cross section was only measured down to an energy of $E_{\text{cm}} = 1.7$ MeV, but the ratio of excited-state to ground-state contributions was also applied when extrapolating down to the resonance energy. Such a treatment neglects, however, any energy dependence of the branching.

The main requirement which determines whether a statistical model is applicable is a high density of states (at least 10 resonances MeV^{-1}) at the projectile binding energy in the compound nucleus, so that an averaging over resonances becomes meaningful. In our case the alpha binding energy in ^{12}B is 10 MeV and the level density at this energy just fulfills the requirement quoted. First attempts by Malaney & Fowler (1989) were based on approximation formulae (Woosley et al. 1975) to the Hauser-Feshbach model. A statistical model calculation with realistic optical potentials and inclusion of experimentally known excited states was performed by Thielemann et al. (1991). Other approaches were taken by calculations in a microscopic and in a potential model. The GCM result (Descouvemont & Baraffe 1990) is too small by two orders of magnitude at a temperature of $T_9 = 1.0$, due to the fact that the resulting resonance is shifted by nearly 500 keV to too high excitation energies. This approach can, however, give insight into the resonance structure. The more adjustable potential model can describe all resonances due to excitations of the projectile-target system (here α - ^8Li), which form probably the most important doorway states, and gave a total rate enhanced by a factor of 1.5 in comparison to the ground-state rate alone (Rauscher et al. 1992). This agreed within reasonable limits with early experiments (Kubono et al. 1999). The value for the ground-state transition is in agreement with the value determined by Paradellis et al. (1990).

The $^8\text{Li}(\alpha, n)$ rates from the different theoretical approaches are given in Figure 2 for comparison. The result by Descouvemont is unrealistically small due to the incorrect energy shift. For our nucleosynthesis calculations we made use of the theoretical rate by Rauscher et al. (1992), which contains more adjustments to the individual nuclear properties than a global statistical model and is in better agreement with the experiment for low-level densities because it implements individual resonances rather than averages. If the experimental evidence, found by Boyd et al. (1992) beyond astrophysical energies, for a larger ratio of the total rate to the ground-state rate alone (5 rather than 1.5) remains valid also at astrophysical energies, the rate employed here would be too small by roughly a factor of 3. Recent experiments suggest this (Mao et al. 1994). To test the effect of such a change, we also performed a few test calculations with a higher rate.

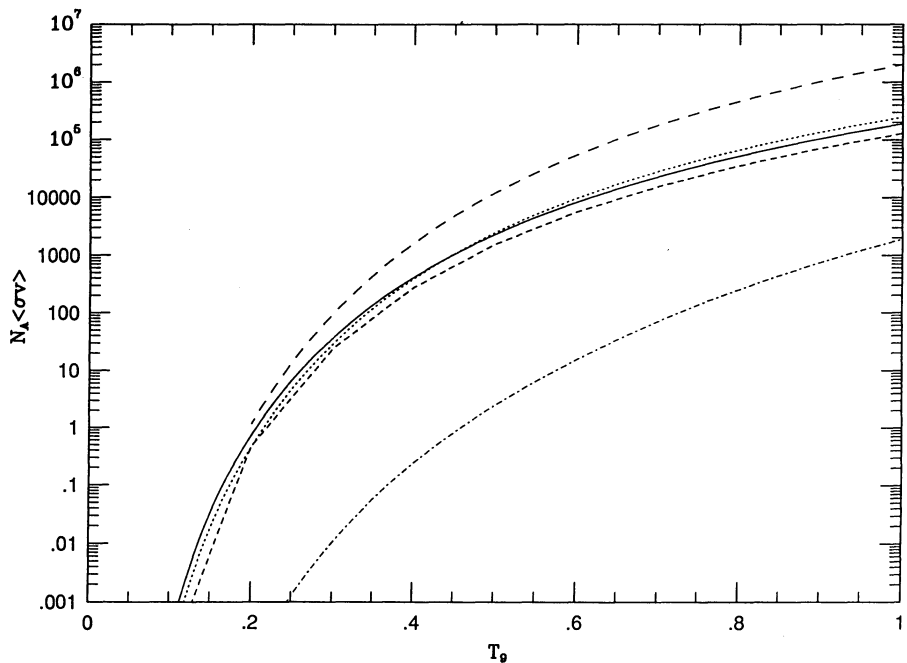


FIG. 2.—Comparison of the ${}^8\text{Li}(\alpha, n){}^{11}\text{B}$ rate from several experimental and theoretical sources. (Solid lines: Malaney & Fowler 1989; short-dashed lines: Thielemann et al. 1987; dotted lines: Rauscher et al. 1992; dash-dot lines: Descouvemont & Baraffe 1990; long-dashed lines: Boyd et al. 1992). The rates from different statistical model and potential model predictions as well as the original experimental determination for the transition to the ground state of ${}^{11}\text{B}$ differ by less than a factor of 2.

Besides ${}^8\text{Li}(\alpha, n){}^{11}\text{B}$, inhomogeneous big bang calculations have spurred a number of experimental investigations in neutron and charged particle-induced reactions over the past years, which could extend big bang nucleosynthesis from ${}^7\text{Li}$ —the endpoint in the standard big bang—to intermediate-mass nuclei also by alternative reaction paths (see the discussion at the beginning of this section). We list in Table 1 the new experimental rates incorporated in our reaction network and (α, n) reactions investigated with statistical model and potential model methods. An additional number of proton-induced reactions on proton-rich unstable nuclei (van Wormer et al. 1994) was incorporated as well, although they are not of importance in the present context.

4.2. Neutron-induced Reaction Rates on Unstable Nuclei

The high neutron concentrations in low-density regions might also make neutron captures feasible on light, unstable, neutron-rich targets. Thus, (n, γ) reactions on light nuclei in the range Li–Ne are of key significance in inhomogeneous big bang scenarios. We know that even those involving stable targets in this region of the nuclear chart bear large uncertainties (Bao & Käppeler 1987; Beer et al. 1989), due to their minute cross sections. Presently only a few rates for unstable nuclei are available, and they stem from old estimates (Wagoner, Fowler, & Hoyle 1967; Wagoner 1969, 1973). Level densities at the relatively small neutron separation energies of neutron-rich compound nuclei are large enough for heavy and perhaps also for medium nuclei to justify the use of statistical model calculations. This is absolutely not the case for nuclei lighter than Ne.

For this reason we calculated neutron capture rates for neutron-rich nuclei from Li to Ne, based on experimental information. The reaction rates are determined by resonant contributions from resonant capture into neutron unbound

levels near the neutron threshold of the compound nucleus and by direct capture into low-lying bound states of the final nucleus $\langle\sigma v\rangle = \langle\sigma v\rangle_{\text{res}} + \langle\sigma v\rangle_{\text{dc}}$. The resonant reaction rate is estimated only for known states, therefore this contribution may be larger than quoted here if the actual level density is higher than currently known. However, for most of the reac-

TABLE 1
RECENT REACTION RATE DETERMINATIONS

Reaction	Reference
${}^7\text{Li}(n, \gamma){}^8\text{Li}$	Lynn, Jurney, & Raman 1991
${}^7\text{Li}(d, n){}^8\text{Be}$	Boyd, Mitchell, & Meyer 1993
${}^7\text{Li}(d, p){}^8\text{Li}$	Boyd, Mitchell, & Meyer 1993
${}^7\text{Li}(t, n){}^9\text{Be}$	Brune et al. 1991
${}^8\text{Li}(\beta^-){}^2{}^4\text{He}$	Sale et al. 1990
${}^8\text{Li}(p, \alpha n){}^4\text{He}$	Becchetti et al. 1992
${}^8\text{Li}(d, p){}^9\text{Li}$	Balbes et al. 1993
${}^8\text{Li}(\alpha, n){}^{11}\text{B}$	Rauscher et al. 1992
${}^9\text{Li}(\alpha, n){}^{12}\text{B}$	Thielemann et al. 1987
${}^9\text{Be}(t, n){}^8\text{Li}$	Boyd et al. 1992
${}^{10}\text{Be}(\alpha, n){}^{13}\text{C}$	Thielemann et al. 1987
${}^{11}\text{B}(n, \gamma){}^{12}\text{B}$	Wang, Vogelaar, & Kavanagh 1991
${}^{11}\text{B}(\alpha, n){}^{14}\text{N}$	Wang, Vogelaar, & Kavanagh 1991
${}^{11}\text{B}(\alpha, p){}^{14}\text{C}$	Wang, Vogelaar, & Kavanagh 1991
${}^{13}\text{B}(\alpha, n){}^{16}\text{N}$	Thielemann et al. 1987
${}^{13}\text{C}(n, \gamma){}^{14}\text{C}$	Raman et al. 1990
${}^{13}\text{C}(d, n){}^{14}\text{N}$	Brune & Kavanagh 1992
${}^{14}\text{C}(d, n){}^{15}\text{N}$	Brune & Kavanagh 1992
${}^{14}\text{C}(n, \gamma){}^{15}\text{C}$	Beer et al. 1992
${}^{14}\text{C}(p, \gamma){}^{15}\text{N}$	Wiescher, Görres, & Thielemann 1990
${}^{14}\text{C}(\alpha, \gamma){}^{18}\text{O}$	Görres et al. 1993
${}^{15}\text{N}(p, \gamma){}^{16}\text{O}$	Decroock et al. 1991; Kiener et al. 1992
${}^{17}\text{O}(n, \gamma){}^{18}\text{O}$	Koehler & Graff 1991
${}^{17}\text{O}(n, \alpha){}^{14}\text{C}$	Koehler & Graff 1991
${}^{18}\text{O}(n, \gamma){}^{19}\text{O}$	Beer, Käppeler, & Wiescher 1993
${}^{20}\text{F}(\beta^-){}^{20}\text{O}$	Wang et al. 1992
${}^{22}\text{Ne}(n, \gamma){}^{23}\text{Ne}$	Beer et al. 1991

tions the Q -values are very small and only a few resonances are expected to contribute. The resonant rate is determined by the resonance energy, $E_r(\text{MeV})$, and the resonance strength, $(\omega\gamma)_r(\text{MeV})$,

$$\langle\sigma v\rangle_{\text{res}} = 2.56 \times 10^{13} (\omega\gamma)_r A^{-3/2} T_9^{-3/2} \exp(11.605 E_r/T_9). \quad (33)$$

Here A is the reduced mass in atomic mass units. The resonance energy is calculated from the known excitation energies of the unbound levels, and the resonance strength was estimated as described in Wiescher et al. (1986).

In the case of small level densities, direct capture is the dominant reaction mechanism, determining the reaction rates. The cross section $\sigma(E)$ is calculated treating this process as an extranuclear channel electromagnetic transition between the continuum wave function of the target-projectile system and the final bound state in a Woods-Saxon potential. Details are described by Wiescher, Steininger, & Käppeler (1989b). The reaction rate for s -wave neutron capture is constant because of the $1/v$ cross section dependence. Here we have taken into account that the neutron direct capture, on neutron-rich light isotopes with a closed p -shell, populates predominantly low-lying excited states with a predominant sd configuration. Therefore, the $E1$ direct capture to these states is characterized by p -wave neutron capture only. With the approximation for the p -wave

neutron penetrability $P_1 = \mu^{1/2} E^{3/2}$, the cross section can be expressed by $\sigma(E) = S_n(\mu E)^{1/2}$, S_n being the S -factor for p -wave neutrons. Then the reaction rate has the form

$$\langle\sigma v\rangle_{\text{dc},p} = 1.787 \times 10^{-16} S_n(\text{barns MeV}^{-1/2}) T_9 \text{ cm}^3 \text{ s}^{-1}. \quad (34)$$

Using this formalism for p -wave capture and the formalism for s -wave capture as described in Fowler et al. (1967), we calculated the total direct capture contribution. The sum of direct capture and resonant terms results in the expressions given in Table 2. This is an enhanced and revised version of Table 2 in Thielemann et al. (1991).

5. RESULTS FOR THE LOW-DENSITY ZONES

The aim of the present investigation was to explore the full consequences of inhomogeneous big bang scenarios to the production of heavy elements in the neutron-rich low-density regions. Only in neutron-rich environments if at all, is it possible, to produce heavy elements. High-density, proton-rich environments might produce some intermediate elements via the triple-alpha reaction but will in no case be able to produce heavy elements beyond Fe.

Full network calculations as described in §§ 2 and 3 were performed, utilizing the temperature relation of equation (2), the density relations of equations (3) and (6), and the initial

TABLE 2
REACTION RATES FOR LIGHT TARGETS

Reaction	$N_A \langle\sigma v\rangle$
$^7\text{Li}(n, \gamma)^8\text{Li}$	$6.288\text{E}+3 + 4.26\text{E}+3/t932 * \exp(-2.576/t9)$
$^8\text{Li}(n, \gamma)^9\text{Li}$	$3.260\text{E}+3 + 6.328\text{E}+4/t932 * \exp(-2.866/t9)$
$^9\text{Be}(n, \gamma)^{10}\text{Be}$	$1.01\text{E}+3 + 1.01\text{E}+4/t932 * \exp(-6.487/t9)$ $+ 5.41\text{E}+4/t932 * \exp(-8.471/t9)$
$^{10}\text{Be}(n, \gamma)^{11}\text{Be}$	$5.96\text{E}+2 + 6.67\text{E}+5/t932 * \exp(-14.85/t9)$
$^{11}\text{Be}(n, \gamma)^{12}\text{Be}$	$3.56\text{E}+2$
$^{11}\text{B}(n, \gamma)^{12}\text{B}$	$7.38\text{E}+2 + 3.86\text{E}+3/t932 * \exp(-0.244/t9) + 3.34\text{E}+4/t932 * \exp(-4.99/t9)$
$^{12}\text{B}(n, \gamma)^{13}\text{B}$	$1.700\text{E}+3 + 9.548\text{E}+3/t932 * \exp(-1.625/t9)$ $+ 1.562\text{E}+3/t932 * \exp(-2.669/t9) + 1.163\text{E}+4/t932 * \exp(-5.919/t9)$
$^{13}\text{B}(n, \gamma)^{14}\text{B}$	$1.02\text{E}+1 + 4.950\text{E}+1 * t9 + 4.940\text{E}+4/t932 * \exp(-4.76/t9)$
$^{11}\text{C}(n, \gamma)^{12}\text{C}$	$3.18\text{E}+4 + 3.30\text{E}+3/t932 * \exp(-0.917/t9) + 1.05\text{E}+6/t932 * \exp(-5.57/t9)$
$^{11}\text{C}(n, \alpha)^8\text{Be}$	$1.66\text{E}+8 + 2.47\text{E}+6/t932 * \exp(-0.917/t9) + 7.55\text{E}+9/t932 * \exp(-5.57/t9)$
$^{11}\text{C}(n, p)^{11}\text{B}$	$2.00\text{E}+8 + 1.60\text{E}+8/t932 * \exp(-0.917/t9) + 8.96\text{E}+9/t932 * \exp(-5.57/t9)$
$^{13}\text{C}(n, \gamma)^{14}\text{C}$	$1.82\text{E}+2 + 4.633\text{E}+4/t932 * \exp(-1.636/t9)$
$^{14}\text{C}(n, \gamma)^{15}\text{C}$	$7.80\text{E}+2 * t9 + 2.05\text{E}+3/t932 * \exp(-21.14/t9)$
$^{15}\text{C}(n, \gamma)^{16}\text{C}$	$5.27\text{E}+2 * t9 + 3.28\text{E}+4/t932 * \exp(-21.56/t9)$
$^{16}\text{C}(n, \gamma)^{17}\text{C}$	$3.66\text{E}+2 * t9$
$^{13}\text{N}(n, \gamma)^{14}\text{N}$	$1.13\text{E}+0 + 2.65\text{E}-2/t932 * \exp(-2.99/t9)$
$^{13}\text{N}(n, p)^{13}\text{C}$	$6.22\text{E}+8 + 6.63\text{E}+5/t932 * \exp(-2.99/t9)$
$^{15}\text{N}(n, \gamma)^{16}\text{N}$	$4.64\text{E}+3 * t9 + 2.04\text{E}+3/t932 * \exp(-9.98/t9)$
$^{16}\text{N}(n, \gamma)^{17}\text{N}$	$1.18\text{E}+2 + 5.75\text{E}+2 * t9 + 4.756\text{E}+3/t932 * \exp(-2.29/t9)$
$^{17}\text{N}(n, \gamma)^{18}\text{N}$	$2.91\text{E}+2 * t9$
$^{18}\text{N}(n, \gamma)^{19}\text{N}$	$3.23\text{E}+2 * t9$
$^{19}\text{N}(n, \gamma)^{20}\text{N}$	$1.54\text{E}+3 * t9$
$^{18}\text{O}(n, \gamma)^{19}\text{O}$	$2.12\text{E}+1 + 5.87\text{E}+3 * t9 + 4.08\text{E}+4/t932 * \exp(-1.769/t9)$ $+ 9.70\text{E}+4/t932 * \exp(-4.305/t9) + 5.11\text{E}+5/t932 * \exp(-7.265/t9)$
$^{19}\text{O}(n, \gamma)^{20}\text{O}$	$7.32\text{E}+2 * t9 + 9.70\text{E}+3/t932 * \exp(-0.209/t9) + 5.86\text{E}+4/t932 * \exp(-1.741/t9)$
$^{20}\text{O}(n, \gamma)^{21}\text{O}$	$1.22\text{E}+3 * t9$
$^{21}\text{O}(n, \gamma)^{22}\text{O}$	$1.74\text{E}+1 * t9$
$^{21}\text{F}(n, \gamma)^{22}\text{F}$	$2.12\text{E}+2 * t9 + 8.42\text{E}+3/t932 * \exp(-0.464/t9) + 1.82\text{E}+3/t932 * \exp(-3.667/t9)$
$^{22}\text{F}(n, \gamma)^{23}\text{F}$	$1.96\text{E}+2 * t9$
$^{23}\text{F}(n, \gamma)^{24}\text{F}$	$3.52\text{E}+3 * t9$
$^{24}\text{F}(n, \gamma)^{25}\text{F}$	$1.20\text{E}+3 * t9$
$^{25}\text{F}(n, \gamma)^{26}\text{F}$	$3.08\text{E}+1 * t9$
$^{23}\text{Ne}(n, \gamma)^{24}\text{Ne}$	$9.53\text{E}+2 + 4.69\text{E}+2 * t9$
$^{24}\text{Ne}(n, \gamma)^{25}\text{Ne}$	$4.93\text{E}+3 * t9$
$^{25}\text{Ne}(n, \gamma)^{26}\text{Ne}$	$7.81\text{E}+2 * t9$
$^{26}\text{Ne}(n, \gamma)^{27}\text{Ne}$	$5.81\text{E}+2 * t9$

neutron and proton mass fractions from equations (7) and (8) for the low-density neutron-rich region 2. Values of η had to be chosen. We made use of the relation between Ω_b and η in equation (4). While the background temperature T_0 is well known, the Hubble constant unfortunately is not, which leaves some uncertainty. With a Hubble constant $H_0 = 62$, i.e., $h_{50} = 1.24$, we obtain $\eta_{10} = 100$ or $\eta = 10^{-8}$ if $\Omega_b = 1$. Four sets of calculations have been performed, employing $\eta_{10,2}$ values of 52, 13, 6.5, and 1.3 [with $\eta_{10} = 64.94\Omega_b h_{50}^2$ and $\eta_{10,2} = (\rho_2/\rho_b)\eta_{10}$]. Earlier calculations explored a range of $5 \leq f_V R \leq 10^4$ (Mathews et al. 1988; Kajino et al. 1990) and found the best fit with primordial abundances of light elements for a combination of $f_V R \approx 10$. This leads to $\rho_2/\rho_b \approx \frac{1}{5}$ (see eq. [6]). Even for $f_V R$ going to infinity, this ratio does not change much, with a lower bound of $\rho_2/\rho_b = X_n = 0.125 = \frac{1}{8}$. The neutron mass fraction in region 2 is bound by $X_{n,2} = 1$ for infinite $f_V R$. We will use this extreme value, i.e., $X_{p,2} = 0$, in order to achieve the highest possible neutron density and the most favorable environment for the formation of heavy elements. With this choice (i.e., $\rho_2/\rho_b = \frac{1}{8}$) the $\eta_{10,2}$ values given above correspond to global η_{10} values of 416, 104, 52, and 10.4. This corresponds to possible choices of (h_{50}, Ω_b) being (2.5, 1), (1.3, 1), (1, 0.8), and (1, 0.16). The range covered in $\eta_{10,2}$ extends from roughly a factor of 2.2 below the lower limit to a factor of 13 above the upper limit for η in the standard big bang. For each of the η -values we considered four different cases of the comoving length scale of the density inhomogeneities d/a (see § 2): (0) ∞ , resulting in negligible neutron back-diffusion; (1) $10^{7.5}$ cm MeV; (2) $10^{6.5}$ cm MeV; and (3) $10^{5.5}$ cm MeV. This is a measure of the size of the low-density region and a function of the volume fraction f_V and the density ratio R in equations (5)–(8). Accordingly, it describes the efficiency of neutron back-diffusion, being dependent on the ratio of surface area to volume, which is larger for small regions.

One might argue that the initial abundances $X_{n,2} = 1$,

$X_{p,2} = 0$ are not the extreme case for producing heavy elements. Under such circumstances, the formation of heavy elements has to wait until some neutrons decay to protons and combine with other neutrons to alpha particles, the stepping-stone to heavier nuclei. With an initial (small) proton abundance, as expected from equation (8) for $f_V R < \infty$, this process could start earlier. The answer is that in any case nucleosynthesis has to wait until the photodisintegration of ^2H ceases. In addition, the extra protons bind more neutrons into alpha particles (He is the dominant element by abundance). These neutrons are missing during the formation of heavy elements from some of the alpha particles. Therefore, less heavy elements are produced when using an initial proton abundance $X_{p,2} > 0$.

5.1. Abundances of Light Elements

In the following we will discuss the details of some calculations, taking the most favorable case for the formation of heavy elements with $\eta_{10} = 416$, corresponding to $\eta_{10,2} = 52$. Here η_{10} denotes the global value and $\eta_{10,2}$ the value in the low-density zone. Figure 3 shows the temperature in units of 10^9 K as a function of time. Figures 4a–4c give the mass fractions of neutrons, protons, and ^4He as a function of time for cases 0, 1, and 2 ($d/a = \infty, 10^{7.5}$, and $10^{6.5}$ cm MeV). The onset of nucleosynthesis takes place after about 200 s at $T \approx 0.1$ MeV $\approx 10^9$ K, when ^2H ceases to photodisintegrate. This is followed by a sudden drop in the neutron density over about 100 s during which most of the primordial nucleosynthesis and the formation of ^4He occur. We see that in the neutron-rich region almost all nucleons end in ^4He . In case 0 (Fig. 4a) this is 90%. Cases 1 and 2 experience increasing efficiency of neutron diffusion, which leads to a reduction in mass by 51% in case 2. The other measurable difference between these runs is the final $^1\text{H}/^4\text{He}$ ratio, which decreases with increasing diffusion efficiency. Almost all protons are destroyed during the synthesis

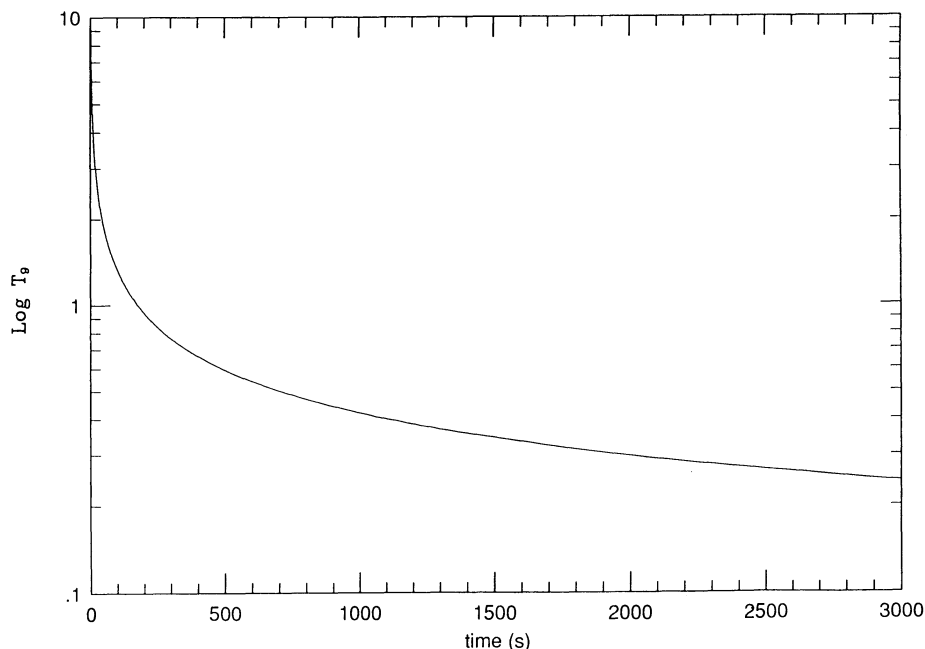


FIG. 3.—Global temperature evolution as a function of time for big bang conditions. Nucleosynthesis and formation of ^2H , ^3He , ^4He , ^7Li , and heavier nuclei set in after the photodisintegration of ^2H ceases at $T \approx 0.1$ MeV $\approx 1.16 \times 10^9$ K and $t = 100$ –200 s.

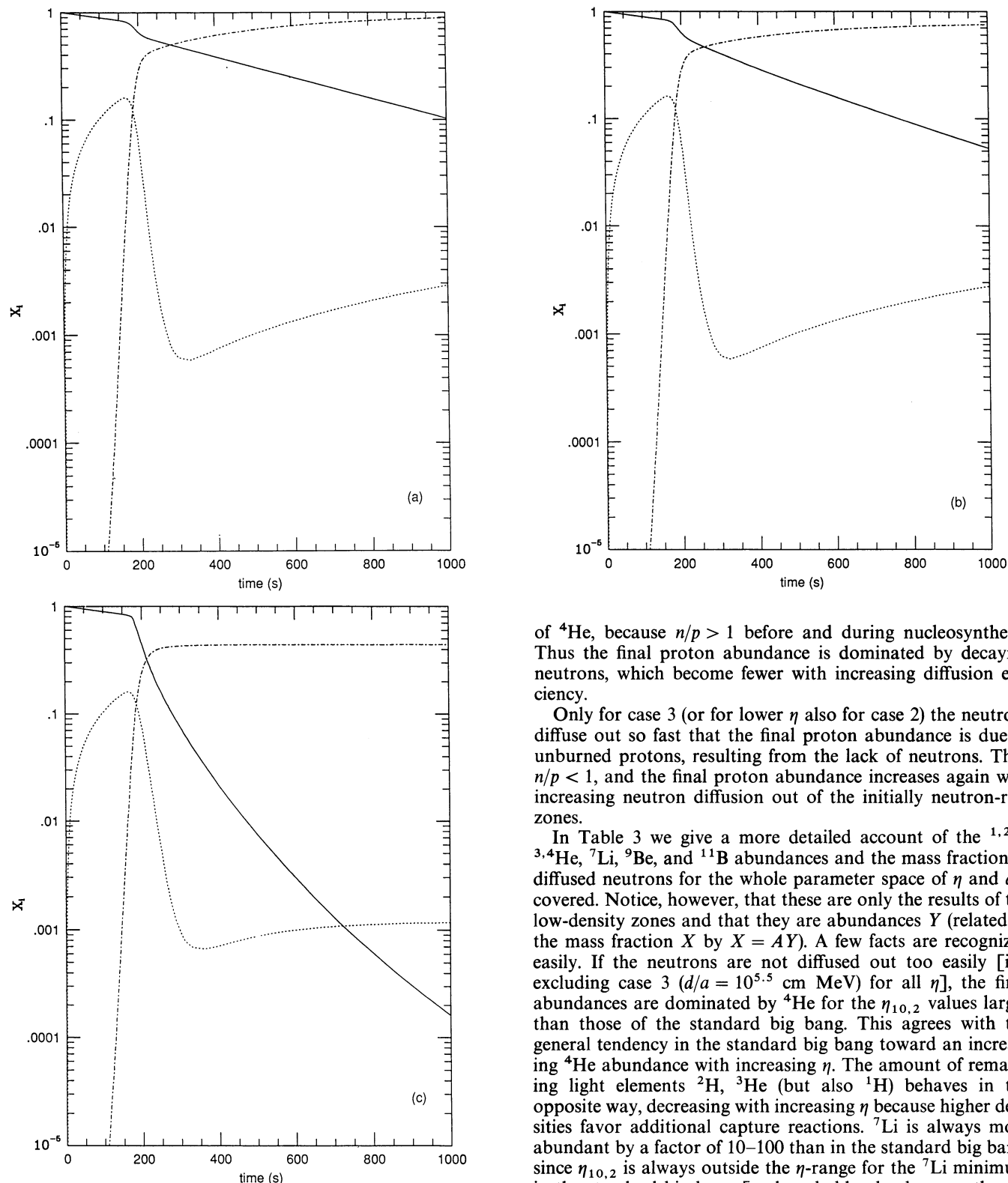


FIG. 4.—Production of light nuclei for $\eta_{10} = 416$, $\rho_2/\rho_b = \frac{1}{8}$ (i.e., $\eta_{10,2} = 52$), representative for $\Omega_b = 1$ and $h_{50} = 2.5$). Only neutrons, protons, and ${}^4\text{He}$ are displayed. Three cases (0, 1, and 2) with varying comoving length scales d/a for the size of the inhomogeneities (which affect the neutron diffusion) are shown: (a) negligible diffusion with $d/a = \infty$ for case 0, (b) $d/a = 10^{7.5}$ cm MeV for case 1, and (c) $d/a = 10^{6.5}$ cm MeV for case 2. All initial protons end in ${}^4\text{He}$; the total mass fraction is dominated by ${}^4\text{He}$; the final proton (${}^1\text{H}$) mass fraction is due to unburned protons from neutron decay and thus dependent on the degree of neutron diffusion losses from neutron-rich zones.

of ${}^4\text{He}$, because $n/p > 1$ before and during nucleosynthesis. Thus the final proton abundance is dominated by decaying neutrons, which become fewer with increasing diffusion efficiency.

Only for case 3 (or for lower η also for case 2) the neutrons diffuse out so fast that the final proton abundance is due to unburned protons, resulting from the lack of neutrons. Then $n/p < 1$, and the final proton abundance increases again with increasing neutron diffusion out of the initially neutron-rich zones.

In Table 3 we give a more detailed account of the ${}^1\text{H}$, ${}^2\text{H}$, ${}^3\text{He}$, ${}^4\text{He}$, ${}^7\text{Li}$, ${}^9\text{Be}$, and ${}^{11}\text{B}$ abundances and the mass fraction of diffused neutrons for the whole parameter space of η and d/a covered. Notice, however, that these are only the results of the low-density zones and that they are abundances Y (related to the mass fraction X by $X = AY$). A few facts are recognized easily. If the neutrons are not diffused out too easily [i.e., excluding case 3 ($d/a = 10^{5.5}$ cm MeV) for all η], the final abundances are dominated by ${}^4\text{He}$ for the $\eta_{10,2}$ values larger than those of the standard big bang. This agrees with the general tendency in the standard big bang toward an increasing ${}^4\text{He}$ abundance with increasing η . The amount of remaining light elements ${}^2\text{H}$, ${}^3\text{He}$ (but also ${}^1\text{H}$) behaves in the opposite way, decreasing with increasing η because higher densities favor additional capture reactions. ${}^7\text{Li}$ is always more abundant by a factor of 10–100 than in the standard big bang, since $\eta_{10,2}$ is always outside the η -range for the ${}^7\text{Li}$ minimum in the standard big bang [and probably also because the n/p ratio is higher and therefore the destruction via ${}^7\text{Li}(p, \alpha){}^4\text{He}$ is reduced]. Thus, in the low-density zone alone, the solar abundances cannot be met.

We list also some small but nonvanishing abundances of ${}^9\text{Be}$ and ${}^{11}\text{B}$. An understanding of their abundances is only possible after the discussion of reaction flows in § 5.2. We can, however, give here an understanding of the trends in Table 3.

TABLE 3
LIGHT-ELEMENT ABUNDANCES Y

$\eta_{10,2}$	d/a	^1H	^2H	^3He	^4He	^7Li	^9Be	^{11}B	X_{diff}
52	0	0.011	4.3E-4	2.5E-6	2.47E-1	4.6E-8	9.9E-13	6.3E-13	0.000
	1	0.008	2.5E-4	1.5E-6	1.98E-1	3.9E-8	5.9E-13	5.9E-13	0.198
	2	0.001	1.1E-5	3.5E-7	1.10E-1	2.6E-8	7.2E-14	2.1E-12	0.557
	3	0.141	6.2E-8	1.7E-7	2.13E-2	6.4E-11	...	1.0E-17	0.774
13	0	0.028	0.4E-4	5.6E-6	2.43E-1	4.9E-8	7.4E-13	2.6E-13	0.000
	1	0.020	5.2E-4	3.0E-6	1.94E-1	4.1E-8	4.6E-13	2.5E-13	0.203
	2	0.018	2.7E-5	1.7E-6	1.02E-1	4.9E-9	1.8E-15	1.5E-14	0.575
	3	0.183	2.6E-8	1.6E-7	5.00E-4	4.1E-13	...	...	0.815
6.5	0	0.045	1.4E-3	8.3E-6	2.38E-1	4.9E-8	6.5E-13	1.7E-13	0.000
	1	0.031	7.6E-4	4.8E-6	1.90E-1	4.1E-8	4.2E-13	1.7E-14	0.203
	2	0.067	4.5E-4	3.7E-6	7.91E-2	1.0E-9	1.7E-16	5.2E-16	0.617
	3	0.184	1.5E-8	2.5E-7	6.52E-5	3.7E-14	...	...	0.816
1.3	0	0.121	3.2E-3	2.0E-5	2.18E-1	4.5E-8	4.8E-13	6.2E-14	0.000
	1	0.085	1.8E-3	1.2E-5	1.72E-1	3.7E-8	3.0E-13	5.9E-14	0.225
	2	0.176	2.3E-4	1.5E-5	2.84E-2	1.0E-9	3.1E-16	8.8E-17	0.710
	3	0.183	2.3E-9	3.1E-7	3.78E-7	5.0E-16	...	...	0.817

Beyond ^7Li , neutrons are the major factor for the formation of heavy elements, starting with $^7\text{Li}(n, \gamma)^8\text{Li}$. More efficient neutron diffusion results in fewer neutrons available for the formation of heavy elements. Therefore, Be is decreasing from case 0 to case 3. The existence of protons hinders the buildup of heavy elements at several locations, e.g., $^7\text{Li}(p, \alpha)^4\text{He}$ and $^{11}\text{B}(p, \alpha)^8\text{He}$. The formation of ^{11}B proceeds via $^8\text{Li}(\alpha, n)^{11}\text{B}$. Here we find two tendencies. The general one is the decrease in the formation of heavy elements with more efficient neutron diffusion. On top of that, we find for $\eta_{10} = 416$ ($\eta_{10,2} = 52$) a slight maximum for case 2. This is due to the fact that the (α, n) reaction ceases early, still at high temperatures. With a higher neutron abundance on long timescales ^{11}B can be further processed via neutron captures. The long existence of neutrons also causes the production of protons on long timescales via neutron decay. These protons can also destroy ^{11}B at late times.

5.2. The Reaction Flow beyond Li

The details of the flow to heavier nuclei beyond Li can be understood when examining Figures 5a and 5b. All of these figures show reaction flows for a global $\eta_{10} = 416$ and $\eta_{10,2} = 52$ in the low-density zones. These are the most favorable conditions for forming heavy elements. The time derivative of each individual abundance $\dot{Y}_i$ in equation (30) is the sum of possible forward and reverse reactions, linking nucleus i with another nucleus j . These can be (n, γ) and the corresponding (γ, n) reactions, (α, n) and (n, α) , etc. That means we can write equation (30) as

$$\dot{Y}_i = -\sum_j f_{ij} = -\sum_j (\dot{Y}_{i,j} - \dot{Y}_{j,i}), \quad (35)$$

where the net fluxes f_{ij} are expressed by the differences between terms of the abundance derivatives of i and j which describe the appropriate reaction from i to j or vice versa. Figures 5a and 5b show the time-integrated fluxes $\int f_{ij} dt$ as arrows, fixed at the point of origin i and pointing toward endpoint j . This means that the angle of the arrow defines the endpoint, which is located along the extension of the arrow. We also combined different reactions with the same origin and endpoint, e.g., β^+ and (n, p) . The normalization is arbitrary. In order to visualize

minor fluxes, orders of magnitude smaller than the dominant ones, a logarithmic normalization was introduced for the length of the vector, $l_{ij} = c/\{1 + [\log_{10}(|f_{ij}/f_{\text{max}}|)]^{3/2}\}$. This normalization also makes smaller fluxes visible, but it means that only slightly longer vectors automatically indicate a dominant flux.

In Figure 5a the maximum flux is passing through $^4\text{He}(t, \gamma)^7\text{Li}$. Other, less important reactions are $^4\text{He}(^3\text{He}, \gamma)^7\text{Be}$ and $^4\text{He}(t, n)^6\text{Li}$, with, however, further reaction links which also end in ^7Li . Major reactions toward heavier nuclei are $^7\text{Li}(n, \gamma)^8\text{Li}$, $^8\text{Li}(\alpha, n)^{11}\text{B}$ or $^7\text{Li}(\alpha, \gamma)^{11}\text{B}$. Large losses back to light elements are due to $^8\text{Li}(\beta^-)^8\text{He}$ [almost comparable to the $^7\text{Li}(n, \gamma)^8\text{Li}$ flux], $^9\text{Be}(p, d)^8\text{He}$ [comparable to the $^7\text{Li}(t, n)^9\text{Be}$ flux], and $^{11}\text{B}(p, \alpha)^8\text{He}$ [comparable to the $^8\text{Li}(\alpha, n)^{11}\text{B}$ flux]. The major flux which leaves the B-chain goes through $^{12}\text{B}(\beta^-)^{12}\text{C}$ with a flux comparable to $^9\text{Li}(\alpha, n)^{12}\text{B}$, a partial branching of the $^8\text{Li}(n, \gamma)^9\text{Li}$ flux. This means that $^9\text{Li}(\alpha, n)^{12}\text{B}$ seems to be now the most efficient rate to process matter beyond Li. The $^9\text{Li}(\alpha, n)^{12}\text{B}$ reaction rate was calculated with the statistical model code SMOKER (see Table 1), while preliminary calculations by Thielemann et al. (1991) were based on only two resonances. Similar to the reaction $^8\text{Li}(\alpha, n)^{11}\text{B}$, the state density is (barely) large enough to allow a statistical model calculation as a close approximation. [If the correct $^8\text{Li}(\alpha, n)$ rate is roughly a factor of 3 higher than the one used here (Boyd et al. 1992), that reaction would again be the dominant one.]

Beyond B, reactions are dominated by neutron and proton captures as well as beta decays. With increasing charge, the proton (and even more so the alpha) captures decrease and neutron captures and beta decays become the major reactions. ^{14}C , having a very long half-life, which makes it stable during big bang nucleosynthesis, has a small neutron capture Q-value of 1.22 MeV. This triggers large photodisintegration reactions of ^{15}C and thus a small net (n, γ) flow. Therefore (see Fig. 5b), the proton capture carries a larger flux, which is, however, comparable to and strongly depleted by $^{15}\text{N}(p, \alpha)^{12}\text{C}$. Furthermore, $^{16}\text{N}(p, \alpha)^{13}\text{C}$ and $^{17}\text{O}(n, \alpha)^{14}\text{C}$ lead to additional depletion, so that the largest flux entering ^{18}O is due to the $^{14}\text{C}(\alpha, \gamma)^{18}\text{O}$ reaction, which suffers some depletion by a comparable flux from $^{18}\text{O}(p, \alpha)^{15}\text{N}$.

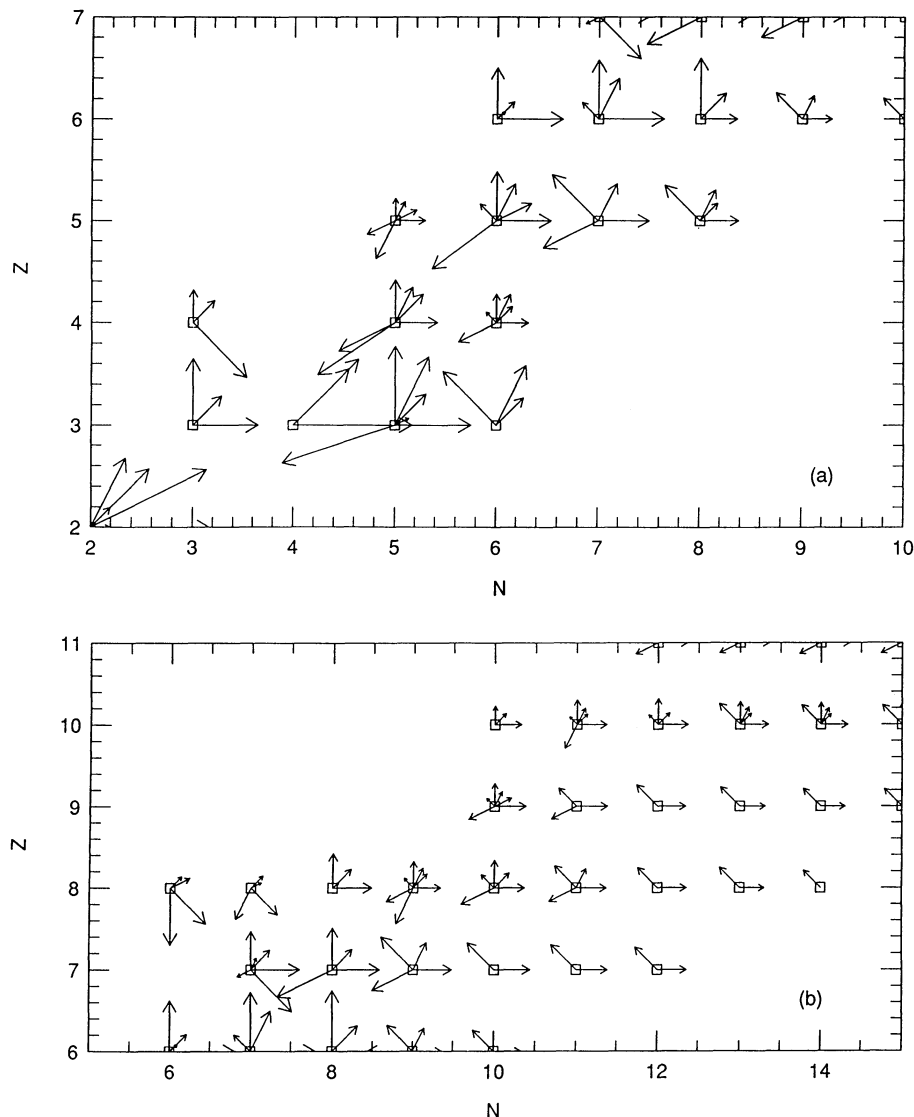


FIG. 5.—Reaction flow pattern for the formation of heavy nuclei. Plotted are the time-integrated fluxes f_{ij} as defined in eq. (35), summed over all reactions which originate at nucleus i and end in nucleus j (see text for the normalization). The arrows start at nucleus i and point in the direction of nucleus j . Shown are the element regions (a) from He to C and (b) from N to Ne. ${}^4\text{He}(t, \gamma){}^7\text{Li}$ and ${}^7\text{Li}(n, \gamma){}^8\text{Li}(\alpha, n){}^{11}\text{B}$ or ${}^7\text{Li}(\alpha, \gamma){}^{11}\text{B}$ are major reactions forming heavier nuclei. The branching ${}^8\text{Li}(n, \gamma){}^9\text{Li}(\alpha, n){}^{12}\text{B}$ seems even more important. Large losses back to light elements are due to ${}^8\text{Li}(\beta^-){}^2{}^4\text{He}$, ${}^9\text{Be}(p, d){}^2{}^4\text{He}$, and ${}^{11}\text{B}(p, \alpha){}^2{}^4\text{He}$. With increasing charge, the proton (and even more so the alpha) captures decrease and neutron captures and beta decays become the major reactions. ${}^{14}\text{C}$ has a small neutron capture Q -value of 1.22 MeV. Large photodisintegration rates cause a small net (n, γ) flow. Therefore, the proton capture has the strongest flux, which is further depleted by (p, α) reactions in the N and O chains. The largest flux into ${}^{18}\text{O}$ is due to ${}^{14}\text{C}(\alpha, \gamma){}^{18}\text{O}$. Beyond O, reactions are dominated by neutron and proton captures and beta decays.

5.3. The Production of Nuclei beyond O

Only beyond O, (p, α) reactions do not form major obstacles any more, and the flow is dominated by (n, γ) reactions and beta decays. The major reaction flow toward heavier nuclei passes through ${}^{20}\text{O}$, ${}^{21}\text{F}$, ${}^{23}\text{Ne}$, ${}^{27}\text{Na}$, ${}^{29}\text{Mg}$, ${}^{31}\text{Al}$, ${}^{34}\text{Si}$, ${}^{37}\text{P}$, ${}^{41}\text{S}$, ${}^{44}\text{Cl}$, ${}^{46}\text{Ar}$, ${}^{49}\text{K}$, ${}^{52}\text{Ca}$, ${}^{53}\text{Sc}$, ${}^{54}\text{Ti}$, ${}^{57}\text{V}$, ${}^{62}\text{Cr}$, ${}^{65}\text{Mn}$, ${}^{66}\text{Fe}$, etc. This reaction path is already located 10 mass units away from stability and will deviate even further for heavier nuclei (see also Thielemann et al. 1991).

The formation of heavy elements is shown in Figure 6 by displaying the mass fractions of several element groups for the same three cases as in Figures 4a–4c. The dashed lines identify elements B–F, the dotted lines Ne–Kr, and the solid lines all elements heavier than Kr. This calculation used the full

network of 655 nuclei from neutrons and protons up to Kr and the r -process network. After 150 s, delayed by about 30–40 s in comparison to ${}^4\text{He}$, B appears together with heavier nuclei. Within another 50 s Ne and heavier nuclei occur due to neutron captures and beta decays. Only 10–15 s later, Kr and heavier nuclei are produced. These decreasing timescales for the buildup of heavier nuclei are caused by smaller neutron capture cross sections and longer beta-decay half-lives of lighter nuclei.

Figures 7a and 7b display the abundances as a function of A from $A = 1$ to $A = 90$ ($Z \leq 36$) for cases 0 and 2 ($\eta_{10,2} = 52$) after beta decay of unstable nuclei. One notices beyond ${}^7\text{Li}$ only one prominent peak at ${}^{14}\text{N}$ due to ${}^{14}\text{C}$ decay. This reflects the fact that ${}^{14}\text{C}$ represents the real bottleneck to heavier ele-

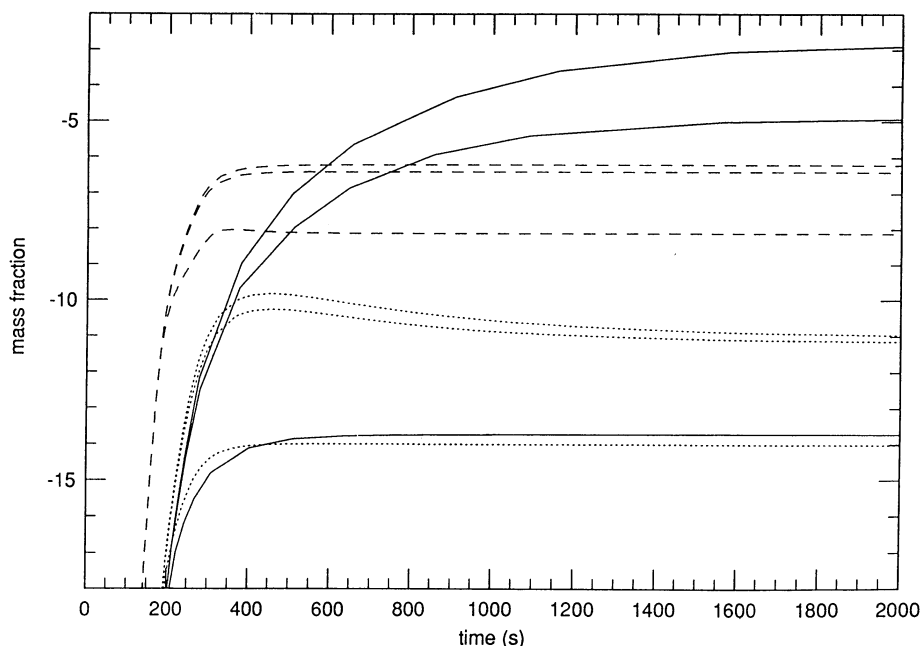


FIG. 6.—Production of heavy nuclei for the same three cases as in Figs. 4a–4c, including only nuclei from B to F (*dashed line*), Ne to Kr (*dotted line*), and beyond Kr (*solid line*). The offset between the three sets of curves indicates that about 50 s are needed to process nuclei from Be to Ne and 10–15 s to process nuclei from Ne to Kr via neutron captures and beta decays. A mass fraction of 10^{-11} of heavy elements is produced for cases 0 and 1 after 350 s. Thereafter the enhancement of *r*-process nuclei depends on the degree of fission cycling, which is negligible in case 2.

ments. Almost all of the (n, γ) and (p, γ) fluxes from ^{14}C are cycled back via (p, α) and (n, α) reactions. Only the strongly Coulomb-suppressed reaction $^{14}\text{C}(\alpha, \gamma)^{18}\text{O}$ allows further processing. The change in d/a or the efficiency of neutron diffusion leads to a decreasing neutron number density n_n and a neutron capture path closer to stability, where longer half-lives are encountered and heavier nuclei are formed with a smaller reaction flux. Even the shift by 1 mass unit can make a tremendous difference when two neighboring nuclei have very different beta-decay half-lives. The abundance at $A = 14$ differs by two orders of magnitude between Figure 7a and 7b (cases 0 and 2). An additional factor of 10 is encountered up to $A = 80$.

5.4. The Big-Bang *r*-Process

For neutron densities in excess of 10^{19} – 10^{20} cm^{-3} , the line in the nuclear chart beyond which beta decay dominates over neutron capture would be located 15–20 mass units away from stability for heavy nuclei. Typical beta-decay half-lives of 10^{-2} to 10^{-3} s are then encountered, with a few exceptions of order 10^{-1} s . Along an *r*-process path at this distance from stability, Fe nuclei can be transformed to U within a few seconds. The transformation from N to Fe takes much longer, however. The actual neutron number densities found in the calculations (shown in Fig. 8) are of order 10^{19} – 10^{20} cm^{-3} between 200 and 300 s for case 0 (but only 10^{18} – 10^{19} cm^{-3} for case 2).

Fission in the *r*-process path can have a strong influence on the total abundances of heavy nuclei as a consequence of “fission cycling,” whereby each of the fission fragments can capture neutrons and finally form again heavy nuclei, which are also prone to fission (Seeger et al. 1965). This is of particular importance in environments with a long duration of high neutron densities, and was therefore suggested as relevant to primordial nucleosynthesis in neutron-rich zones of an inhomogeneous big bang (Applegate 1988). In contrast to the operation of the *r*-process in explosive stellar environments,

confined to a few seconds, this process in the neutron-rich regions associated with an inhomogeneous big bang is only limited by the neutron half-life and can go on for an extended period of time. One of the remarkable features of an *r*-process with fission cycling is that the production of heavy nuclei is not limited to the *r*-process flow (neutron captures and beta decays) coming from light nuclei, but requires only a small amount of fissionable nuclei to be produced initially (a mass fraction of 10^{-11} for cases 0 and 1). One can see the tremendous increase of *r*-process abundances for cases 0 and 1 in Figure 6 after $t = 300 \text{ s}$.

The total mass fraction of heavy nuclei is doubled with each fission cycle and can thus be written as $X_r = 2^n X_{\text{seed}}$. Here n is the number of fission cycles, and X_{seed} denotes the initial mass fraction of heavy nuclei. The main parameter that determines the number of fission cycles is the rate of the *r*-process flux, which is a function of the location of the *r*-process path with respect to the stability line and thus dictates the typical beta-decay half-lives. The location of the *r*-process path is a function of n_n and T , coming closer to stability for decreasing n_n or increasing T (for a general discussion of these *r*-process features see Cowan et al. 1991 and Kratz et al. 1993). Figure 9 shows the nuclear chart with the location of the process path for $n_n = 10^{16}$ – 10^{20} cm^{-3} and a temperature $T = 7 \times 10^8 \text{ K}$. In Table 4 we list the results of test calculations which were performed to determine the fission cycle times τ_{cycl} for $T = 7 \times 10^8 \text{ K}$ as a function of n_n . We notice a tremendous change in τ_{cycl} with decreasing n_n and thus do not expect much cycling once n_n drops down to 10^{17} cm^{-3} at 2000 s (see Fig. 6 for cases 0 and 1). If we consider that for cases 0 and 1 the *r*-process mass fraction at 300 s is equal to those for nuclei in the Ne–Kr range, we need to explain, for cases 0 and 1, $n = 25$ or 16.6 fission cycles until $t = 1000 \text{ s}$. This corresponds to time- (and temperature-) averaged cycle times of 28 and 42 s, which is consistent with Table 4, when considering the neutron den-

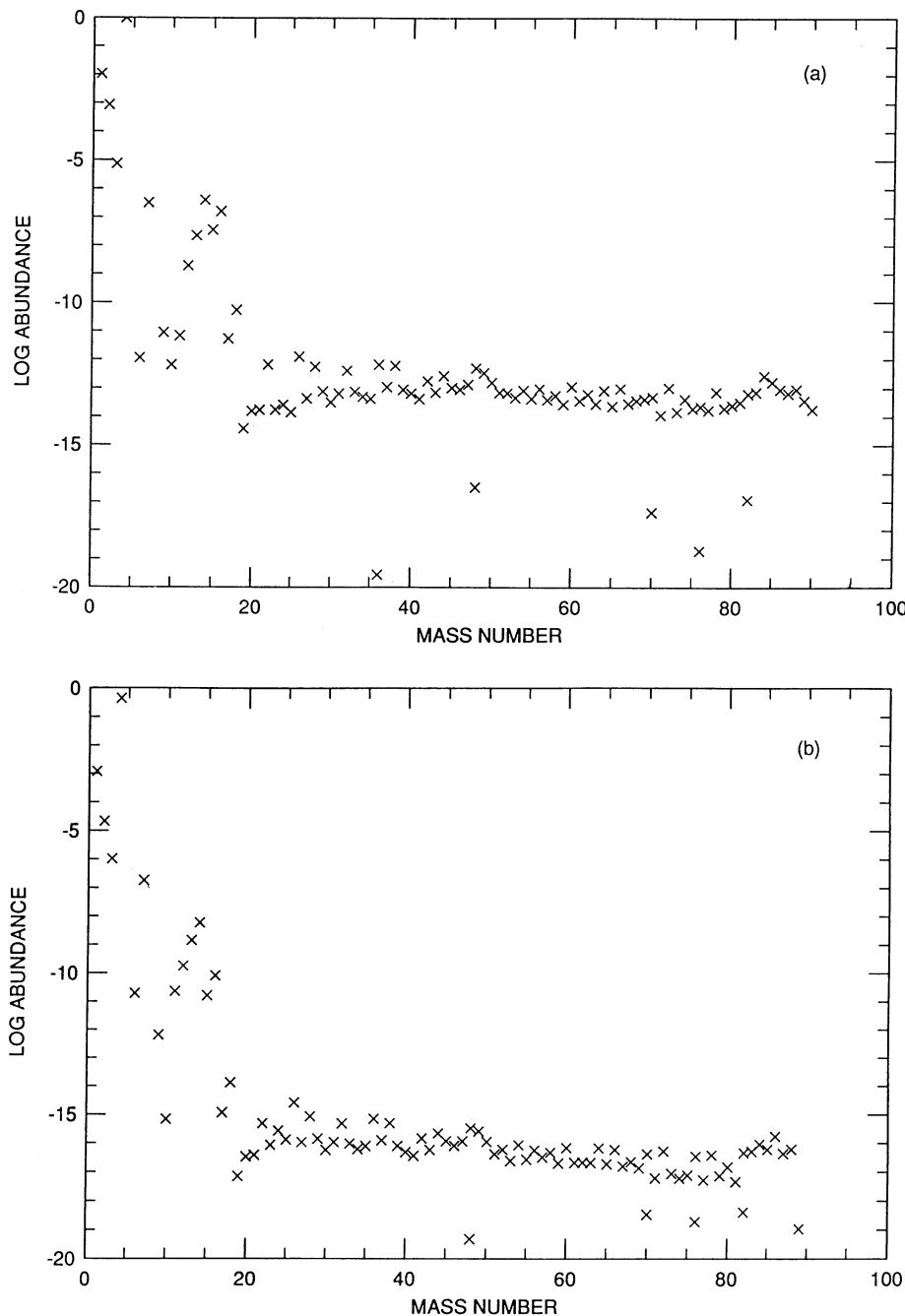


FIG. 7.—Abundances as a function of A from $A = 1$ to $A = 90$ for $\eta_{10,2} = 52$. One notices the prominent peak at ^{14}C , caused by the necessity of charged particle reactions to transport the reaction flow beyond $A = 14$. (a) Case 0; (b) case 2. The change in n_n leads to a neutron capture path closer to stability with longer beta-decay half-lives. In comparison with the results of case 0, the abundances are smaller by two orders of magnitude at $A = 14$ and another factor of 10 up to $A = 80$.

sities of Figure 8 and temperatures of Figure 3. It is also understandable that case 2 experiences essentially no fission cycling at all.

Figures 10a–10c show the abundances for the same three cases at $t = 3000$ s, resulting from the full r -process network beyond Kr. In Figures 10a and 10b one notices that fission cycling was indeed effective, due to the fact that there is a sharp drop visible in abundances just below the $A = 130$ peak. This is the point where fission feeds back with a larger rate than the flow from lighter nuclei and produces a discontinuity. One also

TABLE 4
FISSION CYCLE TIMES

n_n (cm^{-3})	τ_{cycl} (s)
10^{20}	2.84×10^0
10^{19}	1.16×10^1
10^{18}	3.46×10^1
10^{17}	3.73×10^2
10^{16}	2.23×10^3

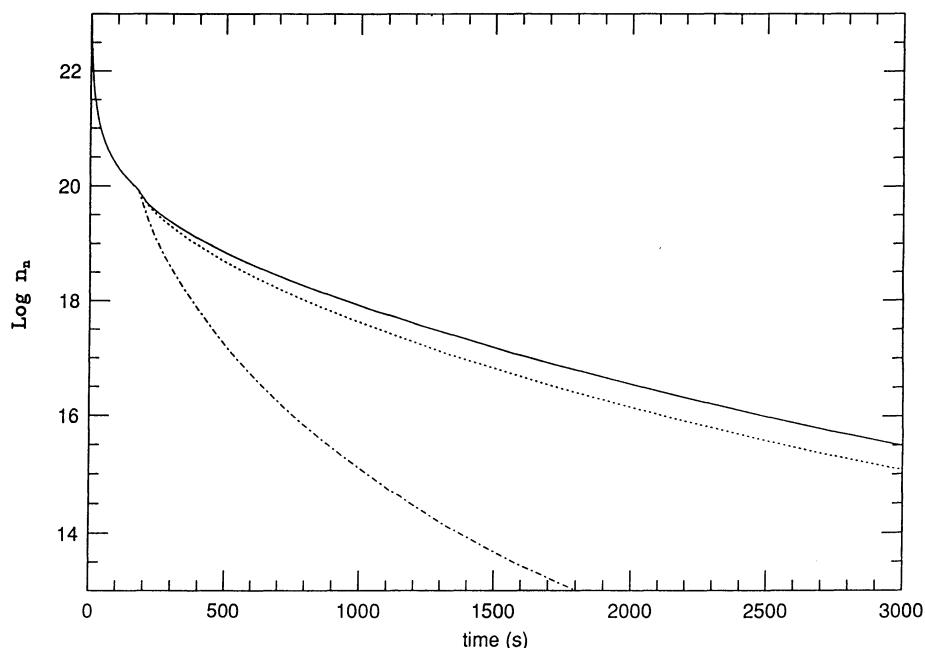


FIG. 8.—Neutron number density n_n in low-density (neutron-rich) regions of an inhomogeneous big bang with $\eta_{10,2} = 52$. The drop after 200 s corresponds to the onset of nucleosynthesis. The three curves represent cases 0, 1, and 2 with different length scales d/a of the density inhomogeneities leading to different efficiencies of neutron back-diffusion. For the first 500 s the number densities are close to r -process conditions for cases 0 and 1.

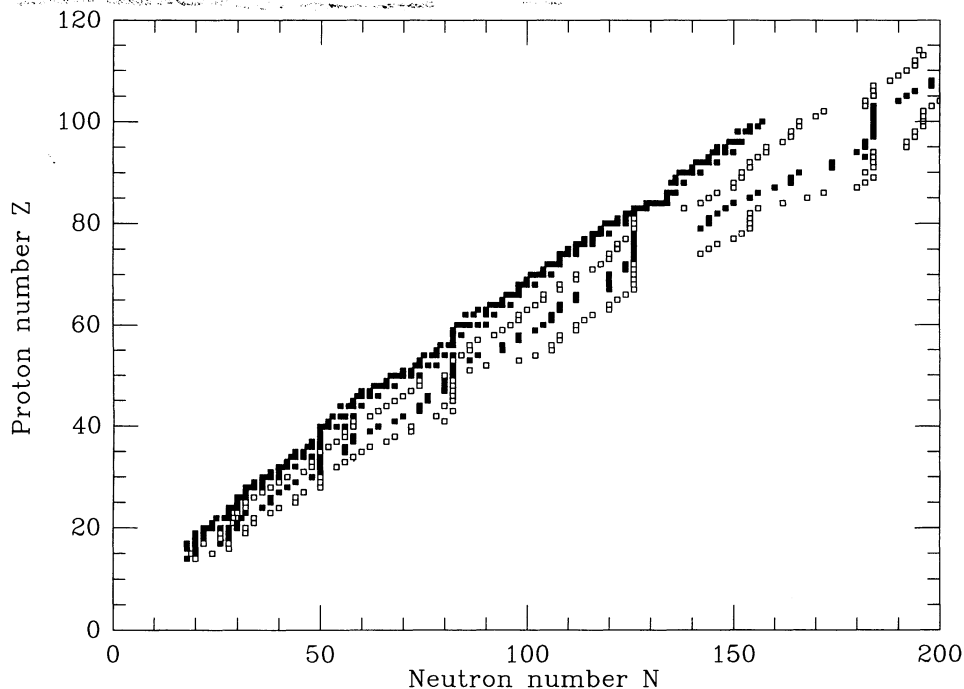


FIG. 9.—Positions of maximum abundances in each isotopic chain (r -process path) for $T = 7 \times 10^8$ K as a function of neutron number density. The filled squares to the left indicate the valley of beta stability. Three sets with increasing neutron number N show the position of the r -process path for three neutron number densities ($n_n = 10^{16}$ [open squares], 10^{18} [filled squares], and 10^{20} [open squares]). Abundance peaks occur at magic neutron numbers (50, 82, 126), where the longest beta-decay half-lives are encountered. The path for $n_n = 10^{16}$ cm $^{-3}$ comes close to the stability valley. That explains the tendency that the abundance peaks move toward higher mass numbers with decreasing n_n (as a function of time in an actual calculation). We expect this to coincide almost with s -process peaks, rather than r -process peaks, at the end of the primordial nucleosynthesis period.

sees that in Figure 10a the final abundances are a factor of 10,000 larger than solar abundances, plotted as triangles. Case 1 shows a result still a factor of 100 above solar, and case 2 is already down to 10^{-7} times solar. When normalizing to global abundances of high- and low-density zones, one has to recognize that $\rho_b = 8\rho_2$ and these results have to be divided by a factor of 8.

An additional feature, not considered so far, becomes obvious in Figures 10a–10c. The abundance peaks do not coincide with *r*-process peaks, but are shifted to higher *A*, almost coinciding with *s*-process peaks. For an initial neutron density of $10^{19} \text{ g cm}^{-3}$, the *r*-process path closely approximates a path reproducing the solar *r*-process abundance pattern (see also Thielemann et al. 1991), but the small neutron densities at late

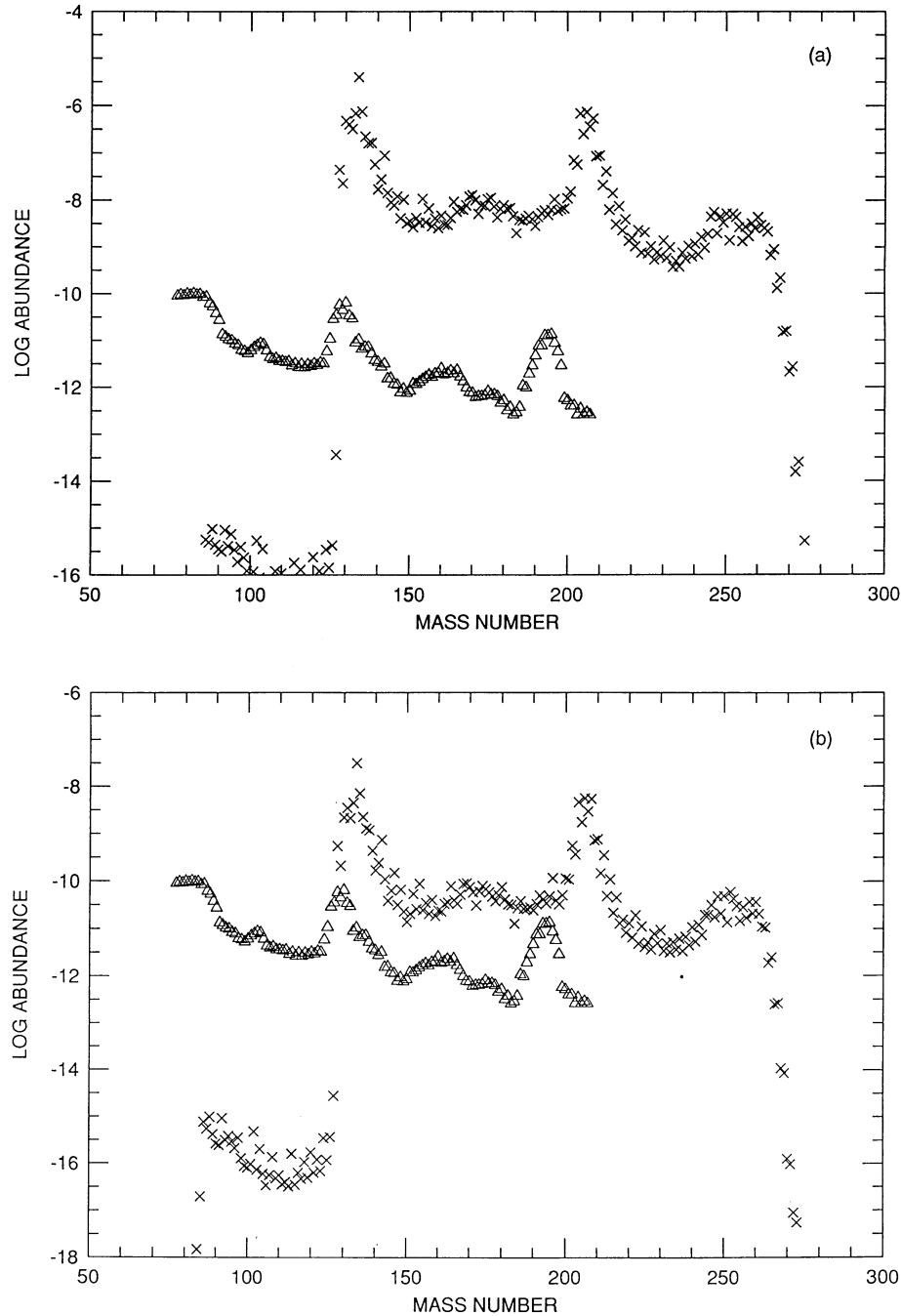


FIG. 10.—Heavy-element abundances due to *r*-process production. Solar *r*-process abundances are indicated by triangles. This is compared with calculations for the low-density region of an inhomogeneous big bang with $\eta_{10,2} = 52$ at $t = 3000$ s. Three cases of inhomogeneous length scales are shown: (a) $d/a = \infty$, i.e., negligible back-diffusion (case 0 of Table 5); the final result is a 10^4 times solar abundance in heavy nuclei within the low-density neutron-rich zone, which has to be divided by 8 in order to obtain the global ratio for high- and low-density zones; the peaks of the nucleosynthesis distributions are shifted to higher values of *A* close to *s*-process positions; (b) $d/a = 10^{7.5} \text{ cm MeV}$; the final abundances are reduced by a factor of 100 in comparison with (a), due to the loss of neutrons via diffusion out of neutron-rich zones (case 1 of Table 5); (c) $d/a = 10^{6.5} \text{ cm MeV}$; the final abundances are reduced by another factor of 10^7 .

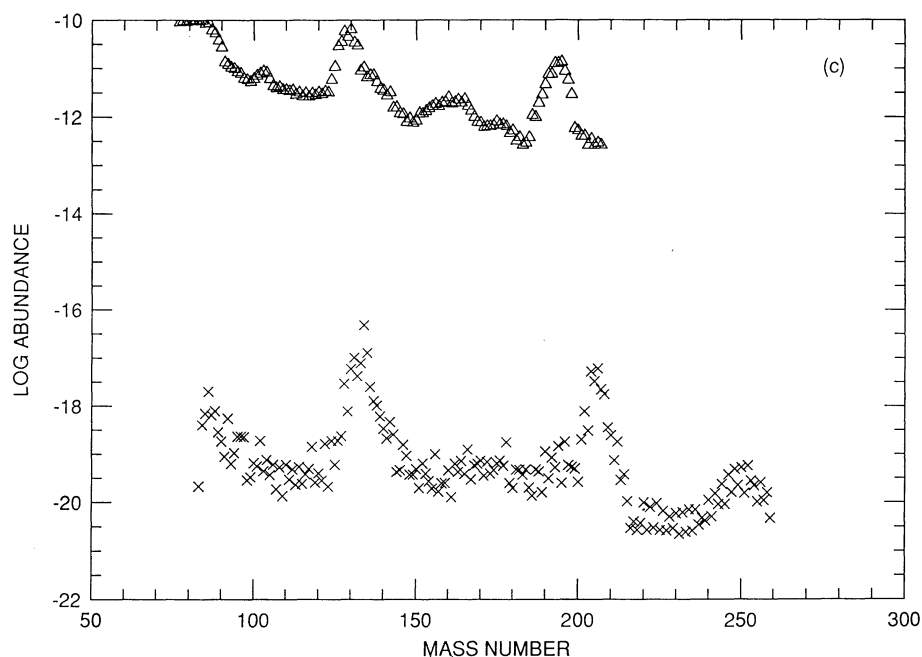


FIG. 10—Continued

time shift the path closer to stability and the abundance maxima to higher A (see Fig. 9). The final positions are closer to s -process peaks than to r -process peaks.

6. RESULTS FOR REALISTIC CONDITIONS AND CONCLUSIONS

This is the first time that the reactions for nuclei above Ne and Si have been included in a calculation for inhomogeneous big bang conditions. In previous studies, their effect was only estimated. The results support the possible mechanism of a big bang r -process brought forward by Applegate (1988). The amount of fission cycling was, however, overestimated in earlier work, as the dependence of the cycle time on density was neglected. When we repeat the same calculation as in Thielemann et al. (1991) for conditions taken from Applegate (1988), with $\eta_{10} = 133$ and $\eta_{10,2} = 16.7$ (note the misprints for the global η and the ρ_2 value in Thielemann et al. 1991), one obtains an average cycle time of 50–70 s rather than the shorter initial estimates. Since the abundances are proportional to 2^n , with n denoting the number of fission cycles, the change to longer cycle times leads to smaller abundance predictions. This is caused by the strongly increasing cycle times with decreasing n , during the expansion (see Table 4) as the (n, γ) path moves closer to the valley of β stability. Nevertheless, the formation of heavy elements beyond Fe and Kr is a very sensitive measure of η [$\eta_{10} = 64.94\Omega_b(H_0/50)^2$] and can provide an independent upper limit for this product of Ω_b and H_0 .

Presently low-metallicity stars from the onset of galactic evolution are known down to $[\text{Fe}/\text{H}] = -4.4$ (Beers, Preston, & Smetman 1992), which corresponds to Fe (and Si) abundances more than 10^4 below solar. The limits on s -process and r -process elements like Sr, Ba, and Eu are known for stars down to $[\text{Fe}/\text{H}] = -3$ with $[(s+r)/\text{Fe}] \approx -1$ (e.g., Mathews, Bazan, & Cowan 1992; Cowan et al. 1991), i.e., these elements are also observed in old stars down to 10^4 below their present values. These low-metallicity observations play the role of an upper limit for primordial nucleosynthesis originating from the big bang.

Case 0, shown in Figure 10a, with $\eta_{10} = 416$ ($\eta_{10,2} = 52$ in the low-density region) or $\Omega_b = 1$, $H_0 = 127$, and $d/a = \infty$, i.e., a very large separation of proton-rich high-density zones, which minimizes the back-diffusion of neutrons out of extended low-density, neutron-rich regions, results in global r -process abundances of about 10^3 times solar ($\approx 10^4$ in the neutron-rich zone). This corresponds to a factor of 10^7 above presently permitted upper limits. For $\eta_{10} = 133$ and $\eta_{10,2} = 16.7$ (equivalent to combinations $\Omega_b = 0.5$, $H_0 = 100$ or $\Omega_b = 1$, $H_0 = 71$), the most favorable case 0 ($d/a = \infty$) results in a factor of 10^3 below solar in the low-density region (shown in Fig. 11), to be divided by another factor of 8 for obtaining the global ratio. This corresponds almost exactly to the presently existing upper limit for primordial r -process abundances.

Table 5 lists the results for all calculations with varying η and d/a . The value $\eta_{10} \approx 104$ or $\eta_{10,2} \approx 13$ [corresponding to $\Omega_b = 1$ and $H_0 = 63$ (or $\Omega_b = 0.4$ and $H_0 = 100$)] leads to predictions which are about a factor of 27 below the present upper limits, whereas for $\eta_{10} = 52$, $\eta_{10,2} = 6.5$ (e.g., $\Omega_b = 0.2$, $H_0 = 100$) the factor is as high as 10^5 . This underlines the very strong and sensitive dependence of primordial r -process abundance on η . Elements like Si and Fe show a much smaller η -dependence. The solar abundances of Si and Fe are 2.7×10^{-5} and 2.4×10^{-5} , respectively. From Figure 7a we can see that for $\eta_{10} = 416$ (case 0) inhomogeneous big bang nucleosynthesis gives rise to Si and Fe abundances roughly 10^8 below solar or 4×10^3 below the present upper limit ($[\text{Fe}/\text{H}] \approx -4.4$) for the primordial abundances of these intermediate elements. This factor changes to 4×10^6 for $\eta_{10} = 104$ and to 4×10^8 for $\eta_{10} = 52$. In neither of these cases do the Si or Fe abundances exceed the upper limit.

Thus, we find that primordial r -process abundances are a very sensitive indicator of η and that for $\eta_{10} = 133$ (i.e., $\Omega_b h_{70}^2 = 2$) r -process abundances equal to the presently observed upper limits for primordial nucleosynthesis can be produced. The amount of heavy elements produced is much more sensitive to η , and with it to the efficiency of fission

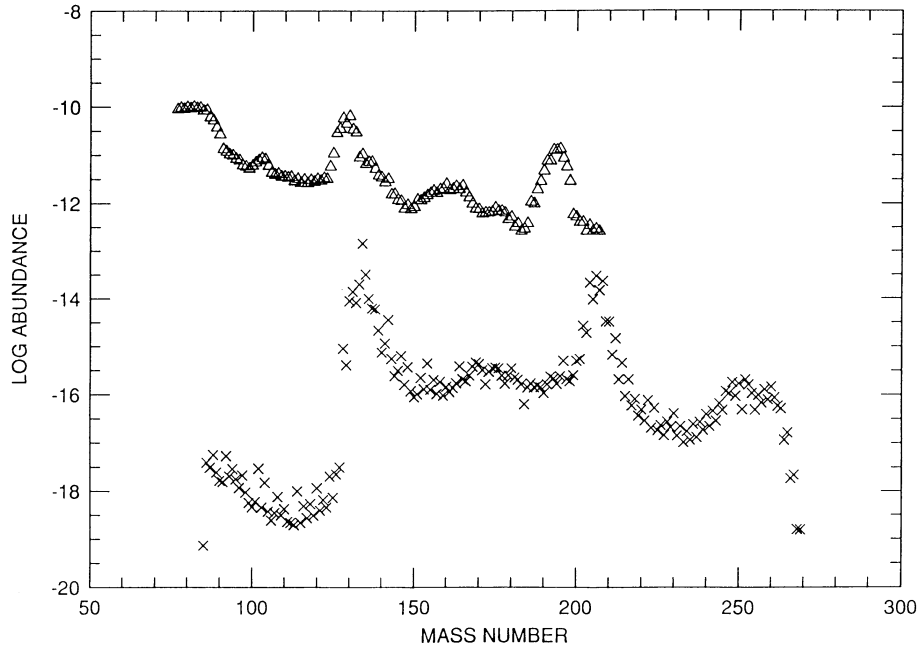


FIG. 11.—Composition for $\Omega_b = 1$, $H_0 = 72$ ($\eta_{10} = 133$, $\eta_{10,2} = 16.7$) and $d/a = \infty$, i.e., negligible neutron back-diffusion at 3000 s. Fission cycling was effective by producing a final mass fraction of heavy nuclei of 6.2×10^{-11} . The abundances are about a factor of 1000 smaller than solar, which has to be diluted by another factor of 8 to obtain global abundances after mixing with the high-density regions. This is about equal to the lowest r -abundances in low-metallicity stars. The smaller n_s in comparison with Figs. 10a and 10b, resulting from a smaller $\eta_{10,2}$ led to an r -process path closer to stability with enhanced beta-decay half-lives and fission cycling times.

cycling, than to changes in the ${}^8\text{Li}(\alpha, n){}^{11}\text{B}$ reaction rate, one of the two bottlenecks toward heavy nuclei [the other being ${}^{14}\text{C}(\alpha, \gamma){}^{18}\text{O}$]. We have performed two calculations (for $\eta_{10} = 416$ and 52 or $\eta_{10,2} = 52$ and 6.5 from Table 5) with a rate enhanced by a factor of 3 and found in both cases, which represent very different regimes, that the resulting heavy-element abundances vary only linearly with the ${}^8\text{Li}$ rate. This can be understood easily, as the seed production of heavy elements varies linearly with the Li rate, and even for strong fission cycling this behavior is not changed because $X_{\text{heavy}} = X_{\text{seed}} \times 2^n$. The number of fission cycles n is only dependent on the neutron densities and not on the seed production via ${}^8\text{Li}(\alpha, n){}^{11}\text{B}$. While the neutron densities and thus the baryon

density parameter η enter into X_{heavy} via the power n , the Li rate enters only linearly. Thus, our conclusions for constraints on η or $\Omega_b h_{50}^2$ remain essentially unchanged.

While heavy elements can be produced in amounts comparable to the ones seen at the lowest observed metallicities for values of $\eta_{10} > 133$ ($\eta_{10,2} > 16.7$ or $\Omega_b h_{50}^2 > 2$), primordial abundances of light elements lead to tighter constraints with $\Omega_b h_{50}^2 < 0.6$ from He alone (Meyer et al. 1991). This corresponds to $\eta_{10} < 39$ ($\eta_{10,2} < 5$), where the most optimistic case for large length scales of density inhomogeneities gives r -process abundances which are a factor of 10^5 below presently observable limits (see Table 5). Therefore, it appears questionable whether observations of primordial r -process abundances can provide better limits for Ω_b and H_0 than light-element abundances, although the production of heavy elements sets in at η -values which are not excessively larger than the ones found there.

Still smaller numbers ($\eta_{10} < 7$, $\Omega_b h_{50}^2 < 0.1$) are obtained when Li, Be, and B are included (Kurki-Suonio et al. 1990; Ryan et al. 1992; Duncan et al. 1993), which differ not much from the standard homogeneous big bang conditions (see, however, recent doubts on the primordial ${}^7\text{Li}$ abundance by Deliyannis, Pinsonneault, & Duncan 1993). It was hoped that the correct treatment of hydrodynamic pressure waves after pair annihilation would destroy some of the Li and other light elements (Alcock et al. 1990; Mathews et al. 1993a) and ease these constraints, allowing $\eta_{10} < 26$ or $\Omega_b h_{50}^2 < 0.4$. The most recent evaluation of this process, however, indicates that when the detailed hydrodynamic evolution of the fluctuations is properly analyzed, this mechanism is not an efficient destroyer of Li (Jedamzik et al. 1993). Such inhomogeneous big bang studies, which allow for a perfect fit of primordial abundances of light elements, and still produce elements beyond $A = 12$, favor conditions where most of the matter experiences the

TABLE 5

MASS FRACTIONS OF INTERMEDIATE AND HEAVY NUCLEI

$\eta_{10,2}$	d/a	B-F	Ne-Kr	Above Kr
52	0	0.619E-06	0.894E-11	0.170E-02
	1	0.392E-06	0.633E-11	0.133E-04
	2	0.755E-08	0.969E-14	0.190E-13
	3	0.129E-11	0.584E-19	...
13	0	0.158E-07	0.962E-14	0.227E-11
	1	0.866E-08	0.322E-14	0.735E-13
	2	0.479E-11	0.136E-19	...
	3	0.429E-17	...	...
6.5	0	0.206E-08	0.111E-15	0.628E-15
	1	0.992E-09	0.242E-16	0.253E-16
	2	0.283E-12	...	...
	3	0.264E-19	...	...
1.3	0	0.958E-11	0.198E-21	...
	1	0.360E-11	...	...
	2	0.253E-14	...	...
	3	...	...	...

average standard big bang densities and temperatures. Only in tiny high-density pockets, containing less than 2% of the baryons, the production of nuclei beyond Li can take place. This occurs at high densities via the triple-alpha reaction. Such proton-rich conditions will not lead to the production of elements heavier than Si and Fe. This is only possible in the neutron-rich environments discussed in this paper.

Note added in manuscript.—We discussed in the text the effect of a change of the ${}^8\text{Li}(\alpha, n){}^{11}\text{B}$ rate by a factor of 3, which was not reflected in Table 5 or Figures 7, 10, and 11. The new ${}^{18}\text{O}(n, \gamma){}^{19}\text{O}$ rate, already cited and expressed in Tables 1 and 2 but not yet included in the calculations (which still made use of the rate given in Table 1 of Thielemann et al. 1991), has a similar effect. It favors the competition with the ${}^{18}\text{O}(p, \alpha){}^{15}\text{N}$ rate (see Fig. 5b) and increases the flow to heavy elements by a factor of 10. Thus, the combined effect of both rate changes is a factor of 30 in all entries for Ne–Kr and beyond Kr in Table 5. Provided that density fluctuations exist with large scale lengths compared with the neutron diffusion length, the corresponding limits for η_{10} or $\Omega_b h_{50}^2$ change to 104 and 1.6, respectively, at which heavy-element abundances are produced in inhomogeneous big bang models at a level comparable to the ones seen

at lowest observable metallicities. This reduces the difference between the constraints from light and heavy elements, although the light-element constraint is still tighter. It also underlines that not all reactions of importance have yet been fully explored, and future changes can be expected.

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APPENDIX

A1. RESONANT AND NONRESONANT CONTRIBUTIONS TO THE REACTION RATES

The reaction rates for many of the neutron capture reactions necessary for the network calculations are unknown. Because most of the reaction cross sections discussed here are determined by only a few resonances and, possibly, by additional direct capture transitions, a Hauser-Feshbach approach, which requires a large level density in the compound nucleus, seems not to be justified. We therefore estimated the cross section for resonant as well as nonresonant reaction contributions on the basis of currently available information about the nuclear structure of the involved nuclei. The rates proposed here may therefore carry a large uncertainty, first because of the insufficient structure information available and second because of the large uncertainty in the input parameters used for these calculations.

The resonant rate for the discussed reactions is derived by

$$N_A \langle \sigma v \rangle_r = 1.54 \times 10^5 \mu^{-3/2} T_9^{-3/2} \sum_i \omega \gamma_i \exp(-11.605 E_i^{\text{c.m.}} / T_9) \text{ cm}^3 \text{ mole}^{-1} \text{ s}^{-1},$$

with μ as the reduced mass of the target and projectile system (in atomic mass units), $E_i^{\text{c.m.}}$ as the resonance energy (center-of-mass system) in MeV, and T_9 as the temperature in 10^9 K. The resonance strength $\omega \gamma$ (in eV) is defined as

$$\omega \gamma = \frac{2J + 1}{(2j_p + 1)(2j_t + 1)} \frac{\Gamma_{\text{in}} \Gamma_{\text{out}}}{\Gamma_{\text{tot}}},$$

J , j_p , and j_t denoting the spin of the resonance, the projectile, and the target nucleus, respectively; Γ_{tot} is the total width of the resonance level, and Γ_{in} and Γ_{out} are the corresponding partial widths for the entrance and exit channels of the reaction.

For the calculations of the resonance strengths we used experimentally determined values as far as possible. In cases with no available information, the particle widths Γ_p were calculated by

$$\Gamma_p = 3 \frac{\hbar^2}{\mu R^2} P_\ell C^2 S,$$

with μ being the reduced mass in atomic mass units, R the nuclear channel radius, P_ℓ the penetrability of the particle through the Coulomb and orbital momentum barrier, and $C^2 S$ the single-particle spectroscopic factor. The latter were taken from available transfer reaction data. If not known, the spectroscopic factors were estimated for the appropriate shell configuration of the level.

The γ -widths were calculated from the known lifetimes of the states. If no lifetime information for the state was available, the γ -width was estimated by calculating the single-particle γ -transition strengths to the ground state and less excited states of the nucleus. To obtain a reliable estimate for the total γ -width of the level, the calculated single-particle γ -width for a certain multipolarity L , $\Gamma_{\text{sp}}(L)$, is weighted with the mean value for typical γ -ray transition strengths $M_{\text{w.u.}}$ (γ -strength in Weisskopf units) in the corresponding mass range (Endt 1979):

$$\Gamma_\gamma = M_{\text{w.u.}} \Gamma_{\text{sp}}(L).$$

Typical strengths for E1 γ -transitions vary between 10^{-4} and 10^{-2} ; for these estimates we used values between $M_{\text{w.u.}} = 10^{-2.5}$ and $M_{\text{w.u.}} = 10^{-3.5}$. Transition strengths for M1 transitions vary between 10^0 and 10^{-2} ; for our estimates we used values from

$M_{\text{w.u.}} = 10^{-1.5}$ to $M_{\text{w.u.}} = 10^{-0.5}$. For E2 transitions a typical value of $M_{\text{w.u.}} = 10$ has been used. This procedure implies a large statistical uncertainty and is only justified by the complete lack of experimental and theoretical information about the nuclei discussed here. The different resonant reactions are discussed in § A2 of this appendix. The calculated level parameters for the different reactions are listed in Table 6.

The rate for nonresonant contributions to the (n, γ) reactions has been derived taking into account possible direct capture transitions as well as, in few cases, the low-energy tails of broad resonances at higher excitation energies.

We have calculated the cross section for the direct radiative capture using first-order perturbation theory:

$$\sigma_{\text{DC}} = \frac{2E_\gamma}{\hbar^2 c v_i (2j_p + 1)(2j_t + 1)} \sum_{m_i, m_f} |\langle f, m_f | H_{\text{int}} | i, m_i \rangle|^2,$$

where v_i is the relative velocity of the interacting nuclei, c is the speed of light, and j_p, j_t are the initial spins of projectile and target particle, respectively. E_γ is the energy of the emitted γ -radiation. The matrix elements $\langle f, m_f | H_{\text{int}} | i, m_i \rangle$ for the transition between the continuum state of the target-projectile system $|i, m_i\rangle$ and the final bound state $|f, m_f\rangle$ in a Woods-Saxon potential $V(r)$ have been calculated as described by Rolfs (1973), with H_{int} as the Hamiltonian for the interaction between the particles and the electromagnetic field. The internal nuclear structure of the final bound state can be approximated by scaling the calculated cross section with the single-particle spectroscopic factor C^2S of the particular level, which was obtained as described above. The calculations have been done for possible E1, M1, and E2 direct capture transitions; the results showed that in all cases M1 and E2 transitions were negligible.

The reaction rate for s -wave neutron capture is derived following Fowler et al. (1967). Since the cross section follows the $1/v$ law, the reaction rate is constant:

$$N_A \langle \sigma v \rangle_s = N_A (\sigma_t v_t) \text{ cm}^3 \text{ mole}^{-1} \text{ s}^{-1},$$

with σ_t as the thermal cross section for the s -wave neutron capture and $v_t = 2200 \text{ m s}^{-1}$ as thermal neutron velocity. The calculated thermal cross sections for the different reactions are discussed in § A2 of this appendix and listed in Table 7.

In many of the reactions, however, the nonresonant E1 direct capture contribution is dominated by p -wave neutron capture.

TABLE 6
RESONANCE PARAMETERS

Reaction	E_x (MeV)	E_p (MeV)	J^π	Γ_{tot} (eV)	Γ_{in} (eV)	Γ_{out} (eV)	$\omega\gamma$
$^8\text{Li}(n, \gamma)^9\text{Li}$	4.310	0.247	$5/2^-$	$1.0\text{E}+5$	$1.0\text{E}+5$	0.56	0.34
$^9\text{Be}(n, \gamma)^{10}\text{Be}$	7.371	0.559	3^-	$1.57\text{E}+4$	$1.57\text{E}+4$	$6.4\text{E}-2$	$5.6\text{E}-2$
	7.542	0.730	2^+	$6.3\text{E}+3$	$6.3\text{E}+3$	0.48	0.3
$^{10}\text{Be}(n, \gamma)^{11}\text{Be}$	1.778	1.275	$3/2^+$	$1.0\text{E}+5$	$1.0\text{E}+5$	1.88	3.75
$^{11}\text{B}(n, \gamma)^{12}\text{B}$	3.389	0.021	3^-	3.1	3.1	$2.5\text{E}-2$	$2.2\text{E}-2$
	3.759	0.43	2^+	$4.0\text{E}+4$	$4.0\text{E}+4$	$3.0\text{E}-1$	$1.9\text{E}-1$
$^{12}\text{B}(n, \gamma)^{13}\text{B}$	5.024	0.144	$1/2^+$	...	...	$1.5\text{E}-1$	$5.0\text{E}-2$
	5.106	0.226	$5/2^-$	$6.0\text{E}+4$	$6.0\text{E}+4$	$9.0\text{E}-2$	$9.0\text{E}-2$
	5.388	0.508	$3/2^-$	$1.0\text{E}+4$	$1.0\text{E}+4$	$1.0\text{E}-1$	$6.9\text{E}-2$
$^{13}\text{B}(n, \gamma)^{14}\text{B}$	1.38	0.41	3^-	...	...	$3.3\text{E}-1$	$2.9\text{E}-1$
$^{11}\text{C}(n, \gamma)^{12}\text{C}$	18.80	0.079	2^+	$1.0\text{E}+5$	$1.5\text{E}+3$	2.0	$1.9\text{E}-2$
	19.20	0.480	1^-	$1.1\text{E}+6$	$5.0\text{E}+5$	$3.5\text{E}+1$	5.97
$^{11}\text{C}(n, p)^{11}\text{B}$	18.80	0.079	2^+	$1.0\text{E}+5$	$1.5\text{E}+3$	$9.7\text{E}+4$	$9.1\text{E}+2$
	19.20	0.480	1^-	$1.1\text{E}+6$	$5.0\text{E}+5$	$3.0\text{E}+5$	$5.1\text{E}+4$
$^{11}\text{C}(n, \alpha)^8\text{Be}$	18.80	0.079	2^+	$1.0\text{E}+5$	$1.5\text{E}+3$	$1.5\text{E}+3$	$1.4\text{E}+1$
	19.20	0.480	1^-	$1.1\text{E}+6$	$5.0\text{E}+5$	$2.5\text{E}+5$	$4.3\text{E}+4$
$^{15}\text{C}(n, \gamma)^{16}\text{C}$	6.109	1.858	2^+	$2.5\text{E}+4$	$2.5\text{E}+4$	$1.7\text{E}-1$	$2.1\text{E}-1$
$^{13}\text{N}(n, \gamma)^{14}\text{N}$	10.812	0.258	5^+	0.4	$1.4\text{E}-6$	$1.6\text{E}-2$	$1.5\text{E}-7$
$^{13}\text{N}(n, p)^{13}\text{C}$	10.812	0.258	5^+	0.4	$1.4\text{E}-6$	0.4	$3.9\text{E}-6$
$^{16}\text{N}(n, \gamma)^{17}\text{N}$	6.08	0.197	$5/2^+$	$2.1\text{E}+4$	$2.1\text{E}+4$	$4.7\text{E}-2$	$2.8\text{E}-2$
$^{18}\text{O}(n, \gamma)^{19}\text{O}$	4.109	0.152	$3/2^+$	<15	<15	$2.44\text{E}-2$	$1.53\text{E}-2$
	4.328	0.371	$(3/2^+)$	<15	<15	$2.9\text{E}-1$	$5.8\text{E}-1$
	4.582	0.626	$3/2^-$	52 ± 3	52 ± 3	1.53	3.06
$^{19}\text{O}(n, \gamma)^{20}\text{O}$	7.622	0.018	3^-	...	...	$1.0\text{E}-1$	$5.8\text{E}-2$
	7.754	0.150	4^+	...	...	$4.7\text{E}-1$	$3.5\text{E}-1$
$^{21}\text{F}(n, \gamma)^{22}\text{F}$	5.260	0.040	1^+	...	...	$2.0\text{E}-1$	$5.1\text{E}-2$
	5.536	0.316	0^+	...	...	$1.3\text{E}-1$	$1.1\text{E}-2$

TABLE 7
NON-RESONANT CONTRIBUTIONS

Reaction	E_f (MeV)	J^π	l_i	l_f	σ_{therm} (barns)	S_n ($\mu\text{barns}/\sqrt{\text{MeV}}$)
${}^8\text{Li}(n, \gamma){}^9\text{Li}$	0.0 2.69	$3/2^-$ $1/2^-$	s s	p p	$3.4\text{E}-2$ $1.1\text{E}-3$	
${}^9\text{Be}(n, \gamma){}^{10}\text{Be}$	...	...	...	...	$7.6\text{E}-3^a$	...
${}^{10}\text{Be}(n, \gamma){}^{11}\text{Be}$	0.0	$1/2^+$	s	p	$4.5\text{E}-3$	...
${}^{11}\text{Be}(n, \gamma){}^{12}\text{Be}$	0.0	0^+	s	p	$2.7\text{E}-3$	...
${}^{11}\text{B}(n, \gamma){}^{12}\text{B}$	...	...	...	...	5.6^a	...
${}^{12}\text{B}(n, \gamma){}^{13}\text{B}$	0.0	$3/2^-$	s	p	$1.3\text{E}-2$	...
${}^{13}\text{B}(n, \gamma){}^{14}\text{B}$	0.0 0.74 1.86 ^b	2^- 1^- 2^-	p p s	d d ...	 $7.7\text{E}-5$	$4.11\text{E}-1$ $2.53\text{E}-1$...
${}^{11}\text{C}(n, \gamma){}^{12}\text{C}$	0.0 4.44 18.35 ^b	0^+ 2^+ 2^-	s s s	p p ...	$2.4\text{E}-2$ $3.6\text{E}-2$ $1.8\text{E}-1$	
${}^{11}\text{C}(n, \alpha){}^8\text{Be}$	18.35 ^b	2^-	s	...	$1.25\text{E}+3$	...
${}^{11}\text{C}(n, p){}^{11}\text{B}$	18.35 ^b	2^-	s	...	$1.5\text{E}+3$	...
${}^{15}\text{C}(n, \gamma){}^{16}\text{C}$	0.0 1.77 3.03	0^+ 2^+ 0^+	p p p	s d s d		2.70 $9.18\text{E}-1$ $6.07\text{E}-1$ $5.37\text{E}-1$ $1.19\text{E}-1$
${}^{16}\text{C}(n, \gamma){}^{17}\text{C}$	0.0 0.29	$1/2^+$ $5/2^+$	p p p	s d d		2.94 $1.36\text{E}-1$ $2.53\text{E}-1$
${}^{13}\text{N}(n, \gamma){}^{14}\text{N}$	0.0 2.31 3.95 10.812 ^b	1^+ 0^+ 1^+ 1^-	s s s s	p p p ...	$9.04\text{E}-2$ $3.08\text{E}-2$ $3.15\text{E}-2$ 8.38	
${}^{13}\text{N}(n, p){}^{13}\text{C}$	10.812 ^b	1^-	s	...	$4.70\text{E}+3$	...
${}^{16}\text{N}(n, \gamma){}^{17}\text{N}$	0.0 1.37 1.85	$1/2^-$ $3/2^-$ $1/2^+$	p p s	s d p	 $8.89\text{E}-4$	2.63 1.13 1.06 0.39 ...
${}^{17}\text{N}(n, \gamma){}^{18}\text{N}$	0.0 0.121 0.575	1^- 2^- 2^-	p p p	d d d		1.63 0.52 0.45
${}^{18}\text{N}(n, \gamma){}^{19}\text{N}$	0.0 1.12	$1/2^-$ $3/2^-$	p p p	s d s d		0.70 0.29 1.39 0.49
${}^{19}\text{N}(n, \gamma){}^{20}\text{N}$	0.0	2^-	p p	s d		11.52 2.51
${}^{18}\text{O}(n, \gamma){}^{19}\text{O}$	...	...	...	...	$1.60\text{E}-4^a$	52.4^a
${}^{19}\text{O}(n, \gamma){}^{20}\text{O}$	0.0 1.67	0^+ 2^+	p p p	d d s		0.54 1.94 4.15
${}^{20}\text{O}(n, \gamma){}^{21}\text{O}$	0.0	$5/2^+$	p	d	...	11.02
${}^{21}\text{O}(n, \gamma){}^{22}\text{O}$	0.0	0^+	p	d	...	0.16
${}^{21}\text{F}(n, \gamma){}^{22}\text{F}$	0.0 0.26 0.66 1.57 1.97	4^+ 3^+ 2^+ 1^+ 2^+	p p p p p	d d d d d		0.68 0.50 0.33 0.17 0.24
${}^{22}\text{F}(n, \gamma){}^{23}\text{F}$	0.0	$5/2^+$	p	d	...	1.78
${}^{23}\text{F}(n, \gamma){}^{24}\text{F}$	0.0 0.86	3^+ 2^+	p p	s s		18.15 12.86
${}^{24}\text{F}(n, \gamma){}^{25}\text{F}$	0.0	$5/2^+$	p	s	...	10.78
${}^{25}\text{F}(n, \gamma){}^{26}\text{F}$	0.0	1^+	p	d	...	0.28

TABLE 7—*Continued*

Reaction	E_f (MeV)	J^π	l_i	l_f	σ_{therm} (barns)	S_n ($\mu\text{barns}/\sqrt{\text{MeV}}$)
$^{23}\text{Ne}(n, \gamma)^{24}\text{Ne}$	0.0	0^+	p	d	...	0.33
	1.98	2^+	p	d	...	1.38
	3.87	2^+	p	d	...	1.06
	4.76	0^+	p	s	...	1.50
	6.03	1^-	s	p	$7.19\text{E}-3$	...
$^{24}\text{Ne}(n, \gamma)^{25}\text{Ne}$	0.0	$1/2^+$	p	s	...	44.87
$^{25}\text{Ne}(n, \gamma)^{26}\text{Ne}$	0.0	0^+	p	s	...	7.12
$^{26}\text{Ne}(n, \gamma)^{27}\text{Ne}$	0.0	$3/2^+$	p	d	...	5.30

^a Experimentally derived cross section.^b Tail contributions from high-energy resonances.

Therefore, the influence of the orbital momentum barrier for p -wave neutrons has to be taken into account (Wiescher et al. 1990). The astrophysical S -factor can then be redefined for p -wave neutrons by

$$S_n(E)_{\ell=1} = \frac{\sigma(E)}{E^{1/2}},$$

with E the neutron energy and $\sigma(E)$ the corresponding capture cross section. The reaction rate is expressed in terms of $S_n(E)$ by

$$N_A \langle \sigma v \rangle = N_A \left[\frac{8}{\mu \pi (k_B T)^3} \right]^{1/2} \int S_n(E) E^{3/2} \exp \left(-\frac{E}{k_B T} \right) dE.$$

The S -factor is nearly constant over the range of the integrand which has its maximum at an energy $E = 2k_B T$. The energy-dependent S -factor is approximated by the constant value at the peak of the integrand $S_n(E) \approx S_n(2k_B T) \equiv S_n$; this yields for the reaction rate

$$N_A \langle \sigma v \rangle = N_A \left[\frac{8}{\mu \pi (k_B T)^3} \right]^{1/2} S_n \int E^{3/2} \exp \left(-\frac{E}{k_B T} \right) dE.$$

Using the analytical solution of the integral, the reaction rate is proportional to the temperature T and, expressed in the standard notation of Fowler, Caughlan, & Zimmerman (1975), is

$$N_A \langle \sigma v \rangle = (1.08 \times 10^8 / \mu^{1/2}) S_n T_9 \text{ cm}^3 \text{ mole}^{-1} \text{ s}^{-1},$$

with the S -factor S_n in units of barns $\text{MeV}^{-1/2}$. The p -wave direct capture distributions for the different reactions are discussed in detail in § A2 of this appendix; the calculated S -factors S_n are listed in Table 7.

The resulting total reaction rates for the neutron capture reactions,

$$N_A \langle \sigma v \rangle = N_A \langle \sigma v \rangle_s + N_A \langle \sigma v \rangle_p + N_A \langle \sigma v \rangle_r,$$

are listed in Table 2.

A2. REACTIONS

A2.1. $^8\text{Li}(n, \gamma)^9\text{Li}$

The rate for this reaction has been estimated by Malaney & Fowler (1988). The Q -value for this reaction is $Q = 4.063 \text{ MeV}$, and the reaction rate is determined by the resonant contribution from the state at 4.31 MeV and by the direct capture transition to the ground state ($3/2^-$) and the first excited state at 2.69 MeV ($1/2^-$) in ^9Li .

Shell model calculations (van Hees & Glaudemans 1984) suggest a $5/2^-$ spin and parity for the resonance level ($E_r = 0.247 \text{ MeV}$). Because of its large total width, $\Gamma = 100 \text{ keV}$, the resonance strength is determined by the γ partial width, which was estimated to be $\Gamma_\gamma = 0.56 \text{ eV}$ (Malaney & Fowler 1988). The resonance parameters are listed in Table 6.

The direct capture to the ground state ($s \rightarrow p$) and to the first excited state ($s \rightarrow p$) has been calculated as described before (Wiescher et al. 1990). The single-particle spectroscopic factors have been calculated as described by Wiescher et al. (1989b), assuming a similar shell configuration as in the case of the mirror nucleus ^9C . The resulting parameters are listed in Table 7.

A2.2. $^9\text{Be}(n, \gamma)^{10}\text{Be}$

The reaction has a Q -value of 6.812 MeV . The thermal cross section is experimentally known, $\sigma_{\text{therm}} = 7.6 \text{ mb}$ (Mughabghab, Divadeenam, & Holden 1981), and is mainly determined by the direct capture to the ground state (0^+) and the first excited state at 3.368 MeV (2^+) in ^{10}Be . Both transitions are s -wave neutron capture transitions, and the cross section follows the $1/v$ law.

Additional resonant contributions to the reaction rate may come from the two unbound states at $7.371 (3^-)$ and $7.542 \text{ MeV} (2^+)$. The resonance strengths are determined by the γ partial widths of these levels, which are experimentally not known. We estimated

the γ -width by assuming for both levels a predominant $L = 1$ γ -decay to the first excited state at 3.368 MeV (2^+). The calculated single-particle γ -widths for both transitions were weighted with the mean value for typical γ -ray transition strengths in that mass region. The resonance parameters are listed in Table 6.

A2.3. $^{10}\text{Be}(n, \gamma)^{11}\text{Be}$

The reaction has a low Q -value of 0.503 MeV. The reaction rate will mainly be determined by the direct capture to the ground state ($1/2^+$) of ^{11}Be . The second excited state in ^{11}Be at 1.78 MeV [$(3/2, 5/2)^+$] may contribute as d -wave resonance to the reaction rate at higher temperatures.

The total width of the resonance level is $\Gamma = 100$ keV (Ajzenberg-Selove 1990). Adopting $J^\pi = 3/2^+$ for this state, we derived its γ -width by weighting the single-particle M1 transition strength to the ground state with the mean value of observed M1 transition strengths in that mass region. The resulting resonance parameters are listed in Table 6.

We have calculated the direct capture ($s \rightarrow p$) to the ground state in ^{11}Be . The ground state has a predominant single-particle structure ($1p_{1/2}$) and therefore a large spectroscopic factor $C^2S = 0.77$ (Ajzenberg-Selove 1990). The nonresonant cross section for s -wave neutrons follows the $1/v$ law. The direct capture parameters are listed in Table 7.

A2.4. $^{11}\text{Be}(n, \gamma)^{12}\text{Be}$

The Q -value of the reaction is 3.168 MeV. The first unbound level in ^{12}Be is at an excitation energy of 4.56 MeV, too high for an appreciable resonant contribution to the reaction rate.

The direct capture to the ground state (0^+) in ^{12}Be ($s \rightarrow p$) is expected to dominate the reaction rate. We have calculated the cross section, assuming a single-particle spectroscopic factor of $C^2S = 0.5$. The resulting parameters are listed in Table 7.

A2.5. $^{11}\text{B}(n, \gamma)^{12}\text{B}$

The reaction ($Q = 3.370$ MeV) has been investigated experimentally by Imhof et al. (1962). Its thermal cross section was determined to $\sigma_{\text{therm}} = 5.6$ barns, dominated by the s -wave direct transition to the ground state (1^+) and the first excited state at 0.933 MeV (2^+) in ^{12}B . The p -wave direct capture to the second and third excited states in ^{12}B is negligible.

Significant resonance contributions are expected from the threshold state at 3.389 MeV (3^-) and the state at 3.759 MeV (2^+), which correspond to resonances at $E_r = 0.021$ ($\ell = 2$) and $E_r = 0.430$ MeV ($\ell = 1$), respectively. The resonance strengths are calculated from the experimentally known level parameters (Ajzenberg-Selove 1990) and are listed in Table 6.

A2.6. $^{12}\text{B}(n, \gamma)^{13}\text{B}$

The reaction has a Q -value of 4.88 MeV. Several unbound levels at 5.024, 5.106, and 5.388 MeV are known in the compound nucleus ^{13}B (Ajzenberg-Selove 1986), which may contribute in the (n, γ) channel. Spin and parity for these levels are not known, but shell model calculations (van Hees & Glaudemans 1984) suggest a $1/2^+$, $5/2^-$, and $3/2^-$ assignment. The γ -partial widths determine the resonance strengths and are derived from the single-particle transition strengths, as described before, assuming a predominant $L = 1$ γ -decay to the ground state ($3/2^-$). The resonance parameters are listed in Table 6.

It is expected that the nonresonant contribution is dominated by the s -wave direct capture to the ground state ($3/2^-$) in ^{13}B . Shell model calculations (Wiescher et al. 1989b) suggest a fairly large spectroscopic factor of $C^2S = 0.72$ for this level. We have calculated the cross section for that transition, and the results are listed in Table 7.

A2.7. $^{13}\text{B}(n, \gamma)^{14}\text{B}$

The Q -value for this reaction is low, $Q = 0.97$ MeV. The second excited state in ^{14}B at 1.38 MeV (3^-) is expected to determine the reaction rate as a d -wave resonance ($\ell = 2$) at a resonance energy of $E_r = 0.41$ MeV. The resonance strength is determined by the γ partial width, which we estimated from the single-particle transition strength, assuming a predominant E1 ground-state transition. The resulting parameters are listed in Table 6.

The low-energy tail of the broad level at 1.86 MeV (2^-), $\Gamma = 1$ MeV contributes to the nonresonant cross section at lower energies. We have calculated the Breit-Wigner shape of the s -wave resonance ($E_r = 0.89$ MeV) for the partial widths $\Gamma_n \approx \Gamma = 1$ MeV and $\Gamma_\gamma = 43$ meV. The latter is estimated from the single-particle transition strength for an M1 transition to the ground state (2^-) in ^{14}B . The contribution to the reaction rate was derived, by following the $1/v$ law, from the calculated cross section at thermal energies.

The configuration of the two bound levels in ^{14}B , ground state (2^-), and first excited state at 0.74 MeV (1^-) are determined by a single neutron in the d -shell. In an E1 direct capture transition they can therefore only be populated by p -wave neutrons ($p \rightarrow d$). We have calculated the cross section for these transitions, adopting for both levels a spectroscopic factor of $C^2S = 0.5$. Because of the orbital momentum barrier the cross section for p -wave neutron capture does not follow the $1/v$ law but drops rapidly with increasing energy. We have calculated the direct capture contribution to the reaction rate following the procedure outlined in § A1 of this appendix.

A2.8. $^{11}\text{C}(n, \gamma)^{12}\text{C}$; $^{11}\text{C}(n, \alpha)^8\text{Be}$; $^{11}\text{C}(n, p)^{11}\text{B}$

The neutron threshold in the compound nucleus ^{12}C is high, $S_n = 18.722$ MeV; thus the level density in this excitation range is fairly large. Four levels are expected to contribute to the reaction rate. The reaction will resonate via the neutron unbound states at 18.80 (2^+), 19.20 (1^-), and 19.40 MeV (2^-), while the subthreshold state at 18.35 MeV (2^-) may contribute via its high-energy tail above the neutron threshold. All four levels are unbound against proton and alpha decay and show large particle widths in both channels (Ajzenberg-Selove 1990). Experimentally also known from $^{11}\text{B}(p, \gamma)^{12}\text{C}$ experiments are the total widths of the states as

well as the γ partial widths. All parameters are listed in Table 6. This allows us to calculate the resonance strengths of the three neutron unbound states in all three reaction channels, (n, γ) , (n, α) , and (n, p) .

The high-energy tail of the subthreshold state is populated by s -wave neutrons; the neutron capture cross section is therefore expected to follow the $1/v$ law. We have calculated the total cross section for all three reaction channels by weighting the production cross section via neutron capture with the decay probability into the γ -channel or the open particle (α , p) channels, respectively. The results are listed in Table 7.

For the $^{11}\text{C}(n, \gamma)^{12}\text{C}$ reaction we also took into account the possible direct neutron capture to the ground state (0^+) and first excited state at 4.439 MeV (2^+) in ^{12}C . Both transitions are based on s -wave neutron capture, and the cross section follows the $1/v$ law. We have calculated the cross section adopting a single-particle spectroscopic factor of $C^2S_0 = 0.9$ and $C^2S_1 = 0.3$ (Ajzenberg-Selove 1990). The results are listed in Table 7.

A2.9. $^{15}\text{C}(n, \gamma)^{16}\text{C}$

The reaction has a Q -value of 4.251 MeV. The level density of ^{16}C is low in this excitation range (Ajzenberg-Selove 1986). The state at 6.109 MeV (2^+ , 3^- , 4^+) is the only observed neutron unbound level. We have calculated its resonance strength in the (n, γ) channel, adopting $J^\pi = 2^+$, an approximate neutron width of $\Gamma_n \approx 25$ keV (Ajzenberg-Selove 1986), and a γ -width $\Gamma_\gamma = 0.17$ eV, estimated for a predominant M1 transition to the first excited state at 1.77 MeV (2^+). The resonance parameters are listed in Table 6.

The ground state (0^+), the first excited state at 1.77 MeV (2^+), and the second excited state at 3.03 MeV (0^+) have a predominant $(s_{1/2} d_{5/2})$ shell structure, coupling one neutron to the ground state ($2s_{1/2}$) or the first excited state ($1d_{5/2}$) of ^{15}C (Wiescher et al. 1990). The E1 direct capture transition to these states will therefore be determined by p -wave neutron capture ($p \rightarrow d$). We have calculated the cross section for the three transitions adopting single-particle spectroscopic factors of $C^2S_0 = 0.5$, $C^2S_1 = 0.1$, and $C^2S_2 = 0.1$ for the three levels. The resulting direct capture parameters are listed in Table 7.

In addition, an s -wave neutron capture will occur through the high-energy tail of the subthreshold resonance level at 3.03 MeV (0^+). We have calculated this contribution for a 100% E2 γ -decay to the first excited state at 1.77 MeV (2^-), which yields a γ partial width of $\Gamma_\gamma = 1.9 \times 10^{-5}$ eV. This s -wave contribution to the reaction rate is only significant at thermal energies.

A2.10. $^{16}\text{C}(n, \gamma)^{17}\text{C}$

The Q -value for the reaction is rather small, $Q = 0.74$ MeV; this indicates a small level density in the populated excitation range of ^{17}C . Only very limited information about the structure of ^{17}C is available. The first excited state has a reported $J^\pi = 5/2^+$; shell model calculations indicate for the ground state either $J^\pi = 1/2^+$ or $J^\pi = 3/2^+$ (Ajzenberg-Selove 1986). These two levels have a predominant $(s_{1/2} d_{5/2})$ structure; therefore, a p -wave direct capture populating these levels is expected. The cross section parameters, calculated with an assumed spectroscopic factor of $C^2S = 0.1$ for both states, are listed in Table 7.

A2.11. $^{13}\text{N}(n, \gamma)^{14}\text{N}$; $^{13}\text{N}(n, p)^{13}\text{C}$

The neutron threshold in the compound nucleus ^{14}N is at $S_n = 10.554$ MeV; therefore, we expect two levels to contribute to the reactions, the neutron unbound state at 10.812 (5^+) as resonance and the neutron bound state at 10.534 MeV (1^-) via its high-energy tail. Both levels are proton unbound and will therefore contribute to both the p and the γ exit channels.

The γ partial widths and the total widths of both levels are well known (Ajzenberg-Selove 1986). The neutron width of the level at 10.812 MeV (5^+), $\ell_n = 5$, has been calculated to 1.4×10^{-6} eV, adopting a single-particle spectroscopic factor of $C^2S_p = C^2S_n = 0.001$. The resulting resonance strength in both reaction channels is listed in Table 6.

The direct capture contribution in the (n, γ) reaction channel comes from s -wave neutron capture to the ground-state (1^+), the first excited state at 2.31 MeV (0^+), and the second excited state at 3.95 MeV (1^+) in ^{14}N . The calculated cross sections for these three transitions are listed in Table 7.

In addition, an s -wave neutron capture will occur through the high-density tail of the subthreshold resonance level at 10.534 MeV (1^-). The level has a proton width of $\Gamma_p = 140$ keV. We adopted a γ -width $\Gamma_\gamma = 5$ eV, similar to other 1^- states in that excitation range. We have calculated the total cross section for both reaction channels by weighting the production cross section via neutron capture with the decay probability into the γ -channel or the open proton channel, respectively. The results are listed in Table 2.

A2.12. $^{16}\text{N}(n, \gamma)^{17}\text{N}$

The Q -value of the reaction is 5.883 MeV. Several neutron unbound states are known from $^{15}\text{N}(t, p)$ experiments. No information about the structure of these levels is available (Ajzenberg-Selove 1986). We therefore took into consideration only the level at 6.08 MeV to estimate its resonant contribution to the reaction rate. We adopted from shell model calculations (Reehal & Wildenthal 1973) the spin and parity of $J^\pi = 5/2^+$ for the level and estimated a neutron width of $\Gamma_n = 21$ keV assuming a spectroscopic single-particle factor of $C^2S = 0.05$. The γ -width was estimated from the single-particle γ transition strength, assuming an E1 transition to the first excited state at 1.37 MeV ($3/2^-$). The resonance parameters are listed in Table 6.

The direct capture to the ground state ($1/2^-$), the first excited state at 1.37 MeV ($3/2^-$), and the second excited state at 1.85 MeV ($5/2^+$) were calculated. The ground state and first excited state have a predominant $(s_{1/2} d_{5/2})$ structure, and can only be populated by a p -wave neutron capture for an E1 transition. The second excited state has a $(p_{1/2})$ component and can be populated by s -wave neutron capture. We have calculated the cross sections for these three transitions, assuming single-particle spectroscopic factors of $C^2S_0 = 0.5$, $C^2S_1 = 0.1$, and $C^2S_2 = 0.1$. The results are listed in Table 7.

A2.13. $^{17}\text{N}(n, \gamma)^{18}\text{N}$

The reaction has a Q -value of 2.825 MeV (Ajzenberg-Selove 1987). Only little information about the structure of the nucleus is available. No neutron unbound states are known. We therefore calculated only the direct capture to the known neutron bound

states, the ground state (1^-), the first excited state at 0.121 MeV (2^-), and the second excited state at 0.575 MeV (2^-). These three states have a dominant ($d_{5/2}$) component and will therefore be populated by a p -wave neutron capture. We have calculated the cross section for all three transitions, assuming a single-particle spectroscopic factor of $C^2S_0 = 0.5$ for the ground state and $C^2S = 0.1$ for the two excited states. The results are listed in Table 7.

A2.14. $^{18}\text{N}(n, \gamma)^{19}\text{N}$

The Q -value of the reaction is 5.32 MeV; no neutron unbound levels are known, therefore only the direct capture component to the known bound states has been derived. Both for the ground state ($1/2^-$) and the first excited state at 1.12 MeV ($3/2^-$) a spectroscopic factor of $C^2S = 0.1$ has been assumed for the calculation of the cross section. The results are listed in Table 7.

A2.15. $^{19}\text{N}(n, \gamma)^{20}\text{N}$

The reaction has a Q -value of 2.32 MeV. Only the E1 direct capture transition to the ground state (2^-) has been considered. Because of the ($s_{1/2} d_{5/2}$) configuration of the ground state, the cross section was calculated for a p -wave neutron capture with a single-particle spectroscopic factor $C^2S = 0.5$. The results are listed in Table 7.

A2.16. $^{18}\text{O}(n, \gamma)^{19}\text{O}$

The Q -value of the reaction is 3.957 MeV. The thermal cross section is known, $\sigma_{\text{therm}} = 0.16$ mbarns. A recent measurement indicated a strong nonresonant p -wave component, which mainly results from direct capture to the first excited state in ^{19}O (Beer, Käppeler, & Wiescher 1993). We have included this term (see Table 7) in the calculation of the reaction rate. To determine the reaction rate at higher temperatures, we also took into account the possible influence of the level at 4.109 MeV ($3/2^+$). The resonance strength is determined by its γ partial width, which was estimated from its single-particle transition strength. For the γ -decay we assumed an M1 transition to the second excited state at 1.47 MeV ($1/2^+$). The contribution of higher energy resonance levels has also been estimated from previous unpublished experimental results (McLane, Dunford, & Rose 1988) and are listed in Table 6. The resulting resonance parameters are listed in Table 6.

A2.17. $^{19}\text{O}(n, \gamma)^{20}\text{O}$

The Q -value of the reaction is 7.607 MeV. We have calculated the resonance strengths of the two neutron unbound states at 7.622 MeV (3^-) and 7.754 MeV (4^+). The γ partial widths have been estimated by assuming a 100% E1 transition to the first excited state at 1.67 MeV (2^+) and a 100% M1 transition to the second excited state at 3.57 MeV (4^+), respectively. The resonance parameter are listed in Table 6.

The direct capture to the ground state (0^+) and the first excited state at 1.67 MeV was calculated. Single-particle spectroscopic factors of $C^2S_0 = 0.5$ and $C^2S_1 = 0.4$ were adopted for these calculations. The results are listed in Table 7.

A2.18. $^{20}\text{O}(n, \gamma)^{21}\text{O}$

The reaction has a Q -value of 3.740 MeV. No information about the level structure of the compound nucleus ^{21}O is available. Therefore, we calculated only the E1 direct capture transition to the ground state. We assumed a predominant ($d_{5/2}$) shell configuration for this level and $J^\pi = 5/2^+$. The level will therefore be populated by a $p \rightarrow d$ transition. We adopted a single-particle spectroscopic factor of $C^2S_0 = 0.5$. The results are listed in Table 7.

A2.19. $^{21}\text{O}(n, \gamma)^{22}\text{O}$

The Q -value of the reaction is 6.766 MeV. No excited levels are known in the compound nucleus ^{22}O . We therefore calculated only the $p \rightarrow d$ direct capture to the ground state, $J^\pi = 0^+$, in ^{22}O . A spectroscopic factor of $C^2S = 0.2$ was adopted for this level. The resulting parameters are listed in Table 7.

A2.20. $^{21}\text{F}(n, \gamma)^{22}\text{F}$

The reaction has a Q -value of 5.220 MeV. Only limited information about the level structure of the compound nucleus ^{22}F is available. In recent spectroscopic work by Orr et al. (1988) and Clarke et al. (1988), four unbound states at $E_x = 5.26, 5.54, 5.70$, and 6.55 MeV have been observed; no spin and parity assignments were made for these states. Shell model calculations (Clarke et al. 1988), however, indicate a much higher level density in this excitation range. Considering only the first two unbound states, we adopted spin and parity values $J^\pi = 1^+, 0^+$, respectively, from shell model states in this excitation range (Wildenthal, Curtin, & Brown 1983). Assuming a predominant M1 transition to the second excited state at 0.66 MeV and the fourth excited state at 1.57 MeV, we estimated typical γ -widths as described before. The parameters are listed in Table 6.

We also calculated the cross section for the additional nonresonant direct capture transitions to the ground state ($J^\pi = 4^+$) and the four excited states at 0.26 (3^+), 0.66 (2^+), 1.57 (1^+), and 1.97 (2^+). For all states we calculated the $p \rightarrow d$ transitions assuming a typical spectroscopic factor of $C^2S_n = 0.1$. The results are listed in Table 7.

A2.21. $^{22}\text{F}(n, \gamma)^{23}\text{F}$

The reaction has a Q -value of 7.54 MeV. Shell model calculations (Wildenthal et al. 1983) indicate a fairly high level density in this excitation range, but no detailed experimental information is available (Orr et al. 1988). Hauser-Feshbach calculations for deriving the reaction rate therefore seem to be justified.

As a lower limit we have calculated the $p \rightarrow d$ direct capture rate for the transition to the ground state ($J^\pi = 5/2^+$). Because ^{23}F has a closed neutron $d_{5/2}$ shell, we adopted a larger spectroscopic factor of $C^2S_n = 0.4$ for the ground state. The result is listed in Table 7.

A2.22. $^{23}\text{F}(n, \gamma)^{24}\text{F}$

The reaction has a Q -value of 2.68 MeV. Shell model calculations (Wildenthal et al. 1983) indicate only one level in this excitation range, but no experimental information is available.

As a lower limit we have calculated the $p \rightarrow s$ direct capture rate for the transition to the ground state ($J^\pi = 3^+$) and a proposed first excited state at 0.86 MeV ($J^\pi = 2^+$). Because these two states in ^{24}F have a predominant $2s_{1/2}$ neutron configuration, we adopted a large single-particle spectroscopic factor of $C^2S_n = 0.8$ for both levels. The results are listed in Table 7.

A2.23. $^{24}\text{F}(n, \gamma)^{25}\text{F}$

The reaction has a Q -value of 4.28 MeV. Shell model calculations (Wildenthal et al. 1983) indicate only one level in this excitation range, but no experimental information is available.

As a lower limit we have calculated the $p \rightarrow s$ direct capture rate for the transition to the ground state ($J^\pi = 5/2^+$) in ^{25}F . The neutron fills the $2s_{1/2}$ shell; therefore, we adopted a spectroscopic factor of $C^2S_n = 0.4$ for this level. The result is listed in Table 7.

A2.24. $^{25}\text{F}(n, \gamma)^{26}\text{F}$

The reaction has a Q -value of 1.04 MeV. Shell model calculations (Wildenthal et al. 1983) indicate no level in this excitation range.

We have calculated the $p \rightarrow d$ direct capture rate for the transition to the ground state ($J^\pi = 1^+$) in ^{26}F . The state is expected to have a predominant $1d_{3/2}$ neutron shell configuration; therefore, we adopted a spectroscopic factor of $C^2S_n = 0.8$ for this level. The result is listed in Table 7.

A2.25. $^{23}\text{Ne}(n, \gamma)^{24}\text{Ne}$

The reaction has a Q -value of 8.86 MeV. Shell model calculations (Wildenthal et al. 1983) indicate a fairly high level density in this excitation range, but no experimental information is available. Hauser-Feshbach calculations for deriving the reaction rate seem therefore to be justified.

As a lower limit we have calculated the $p \rightarrow d$ direct capture rate for the transition to the ground state ($J^\pi = 0^+$) and the first two excited states at 1.98 MeV (2^+) and 3.87 MeV (2^+) as well as the $p \rightarrow s$ direct capture transition to the state at 4.76 MeV (0^+). Because ^{24}Ne has a closed neutron $d_{5/2}$ shell, we adopted a larger spectroscopic factor of $C^2S_n = 0.3$ for the populated states with the predominant $1d_{5/2}$ and $2s_{1/2}$ configurations. In addition, we calculated a direct capture $s \rightarrow p$ transition to the state at 6.08 MeV, assuming a $1p$ hole configuration with a spectroscopic factor of $C^2S_n = 0.8$. The results are listed in Table 7.

A2.26. $^{24}\text{Ne}(n, \gamma)^{25}\text{Ne}$

The reaction has a Q -value of 4.28 MeV. Shell model calculations (Wildenthal et al. 1983) indicate only two levels in this excitation range, but no experimental information is available.

As a lower limit we have calculated the $p \rightarrow s$ direct capture rate for the transition to the ground state ($J^\pi = 1/2^+$) in ^{25}Ne . Because this state has a predominant $2s_{1/2}$ neutron configuration, we adopted a large single-particle spectroscopic factor of $C^2S_n = 0.8$. The results are listed in Table 7.

A2.27. $^{25}\text{Ne}(n, \gamma)^{26}\text{Ne}$

The reaction has a Q -value of 5.48 MeV. Shell model calculations (Wildenthal et al. 1983) indicate only few levels in this excitation range, but no experimental information is available.

As a lower limit we have calculated the $p \rightarrow s$ direct capture rate for the transition to the ground state ($J^\pi = 0^+$) in ^{26}Ne . Because this state has a predominant $2s_{1/2}$ neutron configuration, we adopted a single-particle spectroscopic factor of $C^2S_n = 0.4$. The results are listed in Table 7.

A2.28. $^{26}\text{Ne}(n, \gamma)^{27}\text{Ne}$

The reaction has a Q -value of 1.76 MeV. Shell model calculations (Wildenthal et al. 1983) indicate only one level in this excitation range.

We have calculated the $p \rightarrow d$ direct capture rate for the transition to the ground state ($J^\pi = 3/2^+$) in ^{27}Ne . The state is expected to have a predominant $1d_{3/2}$ neutron shell configuration; therefore, we adopted a spectroscopic factor of $C^2S_n = 0.8$ for this level. The result is listed in Table 7.

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