Standard big bang nucleosynthesis and primordial CNO abundances after Planck

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Abstract. Primordial or big bang nucleosynthesis (BBN) is one of the three historical strong evidences for the big bang model. The recent results by the Planck satellite mission have slightly changed the estimate of the baryonic density compared to the previous WMAP analysis. This article updates the BBN predictions for the light elements using the cosmological parameters determined by Planck, as well as an improvement of the nuclear network and new spectroscopic observations. There is a slight lowering of the primordial Li/H abundance, however, this lithium value still remains typically 3 times larger than its observed spectroscopic abundance in halo stars of the Galaxy. According to the importance of this “lithium problem”, we trace the small changes in its BBN calculated abundance following updates of the baryonic density, neutron lifetime and networks. In addition, for the first time, we provide confidence limits for the production of $^6$Li, $^9$Be, $^{11}$B and CNO, resulting from our extensive Monte Carlo calculation with our extended network. A specific focus is cast on CNO primordial production. Considering uncertainties on the nuclear rates around the CNO formation, we obtain CNO/H $\approx (5 - 30) \times 10^{-15}$. We further improve this estimate by analyzing correlations between yields and reaction rates and identified new influential reaction rates. These uncertain rates, if simultaneously varied could lead to a significant increase of CNO production: CNO/H $\sim 10^{-13}$. This result is important for the study of population III star formation during the dark ages.

Keywords: big bang nucleosynthesis, first stars, physics of the early universe

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1 Introduction

There are three historical observational evidences for the big bang model: the cosmic expansion, the Cosmic Microwave Background (CMB) radiation and primordial or big bang nucleosynthesis (BBN). Today, they are complemented by a large number of evidences in particular from the properties of the large scale structures (see e.g. [51] for a textbook description). BBN predicts the primordial abundances of the “light cosmological nuclei”: $^4$He, D, $^3$He and $^7$Li that are produced during the first 20 min after the big bang when the Universe was dense and hot enough for nuclear reactions to take place (see e.g. [28, 38, 70] for recent reviews). The comparison of the calculated and observed abundances shows an overall good agreement except for the $^7$Li. The essential cosmological parameter of the model is the baryon to photon ratio, $\eta \equiv n_b/n_\gamma = 2.738 \times 10^{-8} \Omega_b h^2$ (see the appendix) that remains constant during the expansion after the electron-positron annihilation. $\Omega_b h^2$ is now well measured from the angular power spectrum of the CMB temperature anisotropies. A precise value for this, previously free, parameter was provided by the Wilkinson Microwave Anisotropy Probe (WMAP9) satellite, $\Omega_b h^2 = 0.02243 \pm 0.00055$, (“Nine-year (MASTER)”, [33]) while the recent Planck mission updated it to $\Omega_b h^2 = 0.02218 \pm 0.00026$ (“Planck+lensing+WP+highL”, [55]). This value is chosen because it includes all the last cosmological constraints. We calculate here the $^4$He, D, $^3$He and $^7$Li primordial abundances by Monte Carlo, using our extended 424 nuclear reaction network [17], also taking into account the updated value of the neutron lifetime [58]. In standard big bang nucleosynthesis, only traces of other isotopes are produced: $^6$Li, $^9$Be, $^{10}$B, $^{11}$B and CNO. The CNO abundance is of peculiar interest since it may affect Pop III stellar evolution in the first structures of the Universe. The value which could impact this evolution is estimated to be $10^{-11}$ [11] or even as low as $10^{-13}$ (in number of atoms relative to hydrogen, CNO/H) for the less massive stars [27]. In this context, it is important to evaluate carefully the BBN CNO abundance.

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In our previous work [17] we obtained a much lower value CNO/H = 0.7 × 10^{-15} but no upper nor lower limit (see also ref. [37]). In this paper, we use the results of our Monte Carlo calculations i) to estimate the uncertainties on the BBN production of the minor isotopes, and in particular of CNO and ii) analyze the correlations between reaction rates and isotopic abundances to identify potentially important reactions that were not identified in our previous sensitivity analysis. We show that by calculating correlations, we find important reactions that were overlooked in sensitivity studies changing one reaction at a time. This is crucial because the level of the CNO abundance plays a key role in the evolution of the first stars.

2 Primitive observational abundances: update

2.1 \(^4\text{He}, \, \text{D,} \, \text{^3He and} \, \text{^7Li observations}\)

Deuterium is a very fragile isotope, easily destroyed after BBN. Its most primitive abundance is determined from the observation of cosmological clouds at high redshift, on the line of sight of distant quasars. Very few such observations are available [52]. Up to now, the observation of about 10 quasar absorption systems gave the weighted mean abundance of deuterium D/H = (3.02 ± 0.23) × 10^{-5} [49]. However, these individual measurements of D/H show a considerable scatter and it is likely that systematic errors dominate the uncertainties. Recently, Cooke et al. [21, 53] have done new observations of Damped Lyman-\(\alpha\) (DLA) systems at high redshift and made a global reanalysis, including previous observations, that lead to a new mean value of

\[
\frac{D}{H} = (2.53 \pm 0.04) \times 10^{-5}, \tag{2.1}
\]

lower and with a much narrower error bar than in previous determinations.

After BBN, \(^4\text{He}\) is still produced by stars. Its primitive abundance is deduced from observations in \(\text{H} \text{II}\) (ionized hydrogen) regions of compact blue galaxies. The primordial \(^4\text{He}\) mass fraction, \(Y_p\), is obtained from the extrapolation to zero metallicity but is affected by systematic uncertainties [6, 41] such as plasma temperature or stellar absorption. Recently, [7, 8], using a subset of the data set found in Izotov et al. ([40, 42], and references therein) have incorporated new atomic data and updated their recent Markov Chain Monte Carlo analysis; so they have determined the primordial helium abundance by a regression to zero metallicity (however within a narrow range of metallicity),

\[
Y_p = 0.2465 \pm 0.0097 \tag{2.2}
\]

which corresponds to a narrower error bar than previous constraints. This is the value we use to compare with our calculations. Another recent determination of [42], \(Y_p = 0.254 \pm 0.003\) is higher than the [8] value. The difference comes from a different a regression to zero metallicity (the mean value, i.e. with no regression, \(Y_p = 0.2535 \pm 0.0036\) of [8] and the [42] one are in perfect agreement) and differences in the atomic physics involved.

Contrary to \(^4\text{He}\), \(^3\text{He}\) is both produced and destroyed in stars throughout its galactic evolution, so that the evolution of its abundance as a function of time is subject to large uncertainties. \(^3\text{He}\) has been observed in our Galaxy [9], and one only gets a ‘local’ constraint

\[
\frac{\text{\text{^3He}}}{{H}} = (1.1 \pm 0.2) \times 10^{-5}. \tag{2.3}
\]
This observation is consistent with the BBN predicted value, nevertheless, due to these uncertainties related to stellar evolution, it is difficult to use it as a constraint.

Primitive lithium abundance is deduced from observations of low metallicity stars in the halo of our Galaxy where the lithium abundance is almost independent of metallicity, displaying the so-called Spite plateau [66]. This interpretation assumes that lithium has not been depleted at the surface of these stars, so that the presently observed abundance can be assumed to be equal to the primitive one. The small scatter of values around the Spite plateau is indeed an indication that depletion may not have been very efficient. However, at very low metallicity, on top of a lot of scatter, a slight decrease of Li with metallicity appears. As a consequence the abundance of lithium could be even lower when extrapolating toward zero-metal stars, just after the Big Bang as pointed by [67]. So, considering the Spite plateau, there is a discrepancy between the value \( i \) deduced from these observed spectroscopic abundances and \( ii \) the BBN theoretical predictions assuming \( \Omega_b \) is determined by the CMB observations. Many studies have been devoted to the resolution of this so-called Lithium problem and many possible “solutions”, none fully satisfactory, have been proposed. For a detailed analysis see [28], the proceedings of the meeting “Lithium in the cosmos” [39] and recently [23]. Note that recent lithium observations [34] have been done in the Small Magellanic Cloud which is a nearby irregular galaxy with quarter of the sun’s metallicity and its abundance is found to be nearly equal to the BBN one. It could be a strong constraint for the lithium galactic evolution. Astronomical observations of these metal poor halo stars [60] have thus led to a relative primordial abundance of Li/H = \( 1.23^{+0.34}_{-0.16} \times 10^{-10} \) while a more recent analysis [62] gives

\[
\text{Li/H} = \left(1.58^{+0.35}_{-0.28}\right) \times 10^{-10}
\]  

which we use in our analysis. For reviews on the Li observations, we refer to [67] and [29].

2.2 \( ^6\text{Li}, \ ^9\text{Be}, \text{B, CNO observations} \)

The origin of the light elements LiBeB, is a crossing point between optical and gamma spectroscopy, non thermal nucleosynthesis (via spallation with Galactic Cosmic Rays, GCR), stellar evolution and Big Bang nucleosynthesis. Lithium-6 is also observed in metal poor stars, as discussed above for \( ^7\text{Li} \). Its observational history is peculiar. In the past, [4] have provided observations of \( ^6\text{Li}/^7\text{Li} \) ratio which suggesting the presence of a plateau, at typically \( ^6\text{Li}/\text{H} = 10^{-11} \), leading to a possible pre-galactic origin of this isotope (see [59]). In a second time, the observational \( ^6\text{Li} \) plateau has been questioned in [12] who have considered in more details the line shape asymmetries. Consequently, there has been a retraction concerning the existence of a \( ^6\text{Li}/\text{H} \) plateau [45]. Presently, only one star, HD84937, presents a \( ^6\text{Li}/^7\text{Li} \) ratio of the order of 0.05 (see [68]) and there is no remaining evidence for a plateau at very low metallicity. We hence use this value as an upper limit: \( ^6\text{Li}/\text{H} \leq 10^{-11} \) while the prediction of the BBN calculations are \( ^6\text{Li}/\text{H} = 10^{-14} \).

Beryllium has only one stable isotope \( ^9\text{Be} \). As D and Li, it is a fragile nucleus. It is formed in the vicinity of Type II supernovae (SNII) by non thermal process (spallation) (see [73, 74]). It is also observed in metal poor stars. [10] (and references therein) have performed an update of Be observations in metal poor stars which provides a primitive abundance at very low metallicity of the order of Be/H = 3. \( \times 10^{-14} \) at [Fe/H] = -3.5. This observation, that we adopt as upper limit of the primordial abundance, has to be compared to the typical primordial Be abundance, Be/H = 10^{-18}.

Boron has two stable isotopes: \( ^{10}\text{B} \) and \( ^{11}\text{B} \). It is also synthesized by non thermal processes, GCR or neutrinos (for \( ^{11}\text{B} \)) (see [72, 73, 75]). The most recent observations of
boron in low metal stars come from [26] and [30]. In the galactic halo, the lowest boron abundance at [Fe/H] \( \approx -3 \) is \( B/H \approx 10^{-12} \), to be compared to the typical primordial B abundance \( B/H = 3 \times 10^{-16} \).

For a general review of these light elements, see the IAU Proceedings [13].

Finally, CNO elements are observed in the lowest metal poor stars (around [Fe/H]=-5). The observed abundance of CNO is typically [CNO/H] = -4, relatively to the solar abundance i.e. primitive CNO/H<10^{-7}. For a review see [29] and references therein.

3 Effects of \( \Omega_b h^2 \), \( \tau_n \) changes and network extension

Concerning the update of the CMB, a comparison between the columns of table 1 shows the effect of a change in \( \Omega_b h^2 \) from [64] (column 2) to [43] (columns 3 or 4; depending on the choice of the neutron lifetime) and to [55] (column 5). In that way, we can trace the changes in our previous publications e.g. in [15] where we used three-years WMAP only [64], in [17] (seven-years WMAP [43]) until this work (Planck+lensing+WP+highL [55]), together with evolving Particle Data Group evaluation of the neutron lifetime, over the years. For the final calculations, we choose, for \( \Omega_b h^2 \), the value from the Planck paper that incorporate the Planck temperature data, polarization data from the WMAP satellite in the multipole range \( 2<\ell<23 \), information from the lensing potential as determined from the trispectrum computed on Planck’s maps [56] and information coming from ground-based high resolution experiments, such as ACT and SPT. This data set, referred to as “Planck+lensing+WP+highL” can be considered to the most uptodate combination of CMB data, hence leading to the most accurate estimation of the cosmological parameters. These changes mostly affects \( ^7\text{Li}/H \) by about 4% and \( \text{D}/H \) by about 2.7% while the other changes are below a percent. Even though it won’t change the nature of the “lithium problem”, we found important to trace the small changes in its BBN calculated abundance following updates of the baryonic density, neutron lifetime and networks. A BBN evaluation has been done by [55], using \( \Omega_b h^2 = 0.02207 \pm 0.00027 \); their prediction regarding the \( Y_p \) and \( \text{D}/H \) abundances are similar to ours (0.24725\( \pm \)0.00032 and 2.656\( \pm \)0.067\( \times \)10^{-5} respectively at \( \eta_{\text{CMB}} \)) but they do not provide any \( ^7\text{Li}/H \) value. In table 1, we show the influence of changes in \( \Omega_b h^2 \) and \( \tau_n \) with a minimal network. Table 2, compared to table 1, show the effect of extending the network. Small differences in \( \text{D} \) and \( ^7\text{Li} \) are observed but that could not be traced to well identified origins: as we shall see in section 6, there are combined effects of reaction rates that are different from the effects of individual rates. However, changes in neutron late time abundance and sub-dominant \( ^7\text{Be} \) destruction mechanism like \( ^7\text{Be}(n,\alpha)^4\text{He} \) [79] play a role. Finally, in table 5, we compare our Monte Carlo (section 4.1) results to observations (section 2.1).

Note that in order to precisely compare our \( Y_p \) values with [55] and some other works, an additional \( \Delta Y_p = 0.0018 \) correction should be made. The weak reaction rates [25] that we numerically integrate include zero-temperature Coulomb and radiative corrections [25, 47]. This correction amounts to \( \Delta Y_p = 0.00316 \), in our calculations at the relevant \( \Omega_b h^2 \) (0.0031 in [47]). What we have neglected, up to now are the finite-nucleon mass correction (\( \Delta Y_p = 0.0012 \) [47]), finite-temperature radiative correction (\( \Delta Y_p = 0.0003 \) [47]), QED plasma (\( \Delta Y_p = 0.0001 \) [47]) and neutrino decoupling (\( \Delta Y_p = 0.0002 \) [48]), for a total of \( \Delta Y_p = 0.0018 \), because they cannot be easily directly re-calculated.\(^1\) Hence, our quoted \( Y_p \)

\(^1\)We numerically calculate the weak rates, to keep track on the dependence w.r.t. \( G_F \) (Fermi constant), \( m_e \) (electron mass) and \( Q_{np} \) (neutron-pronton mass difference), essential in our investigations concerning variations of constants in BBN [14, 18].
Table 1. Primordial abundances with reduced network. (Bold face displayed values highlight parameter changes.)

| Nb. reactions | (a) 424 | (b) 424 | This work | This work |
|---------------|---------|---------|-----------|-----------|
| $\Omega_b h^2$ | 0.02243 | 0.02207 | 0.02249  | 0.02249  |
| $\tau_n$     | 880.1   | 880.1   | 880.1     | 880.1     |
| $Y_p^*$       | 0.2475  | 0.2475  | 0.2464    | 0.2464    |
| D/H ($\times 10^{-5}$) | 2.60 | 2.67 | 2.64 | 2.72 |
| $^3$He/H ($\times 10^{-5}$) | 1.05 | 1.05 | 1.06 | 1.06 |
| $^7$Li/H ($\times 10^{-10}$) | 5.13 | 4.96 | 4.98 | 4.98 |

*An additional $\Delta Y_p = 0.0018$ correction should be made (see text). (a) [15]; (b) [17]; (c) [64]; (d) [57]; (e) [43]; (f) [58]; (g) [55]

Table 2. Primordial abundances with extended network.

| Nb. reactions | (a) 424 | (b) 424 | (c) 424 |
|---------------|---------|---------|---------|
| $\Omega_b h^2$ | 0.02207 | 0.02218 | 0.02218 ± 0.00026 |
| $\tau_n$     | 880.1   | 880.1   | 880.1 ± 1.1 |
| $Y_p^*$       | 0.2465  | 0.2463  | 0.2461–0.2466 |
| D/H ($\times 10^{-5}$) | 2.60 | 2.67 | 2.57–2.72 |
| $^3$He/H ($\times 10^{-5}$) | 1.04 | 1.05 | 1.02–1.08 |
| $^7$Li/H ($\times 10^{-10}$) | 5.13 | 4.96 | 4.56–5.34 |

*An additional $\Delta Y_p = 0.0018$ correction should be made (see text). Hinshaw et al., WMAP9 [33] (y) Planck only [55] (z) Planck+lensing+WP+highL [55]

Uncertainties reflect the nuclear uncertainties, mainly $\tau_n$, not the theoretical uncertainties on theses corrections, difficult to estimate for us. Nevertheless, these neglected corrections (i.e. the $\Delta Y_p = 0.0018$ not included in the above tables) remain one order of magnitude below the observational uncertainty: 0.2465 ± 0.0097.

Since the neutron lifetime and baryonic density values are both subject to debate ([58, 80] for $\tau_n$ and [55] and [65] for $\Omega_b h^2$), instead of providing new tabulated values, we propose fits for the BBN abundances of $^4$He, D, $^3$He and $^7$Li abundances as a function of $\Omega_b h^2$, $\tau_n$ and $N_{\text{eff}}$ (see definition below) hence of the BBN predictions. This can be used to update any column of tables 1 and 2 with $\Omega_b h^2$ or $\tau_n$ different values than those in the same column or for $\Delta N_{\text{eff}} = N_{\text{eff}} - 3 \neq 0$. Our motivation is to provide simple fits that could be directly used to calculate the effect induced by the small changes in and $\Omega_b h^2$ or $\tau_n$ until their precise values are settled. Fitted BBN abundances were already provided by e.g [38, 47, 71] but, they $\eta$ instead of $\Omega_b h^2$ [47] (see the appendix), lack $N_{\text{eff}}$ [38] or $\tau_n$ [71]. We checked that, for small variations our results are very close to [38] for $\tau_n$ and $\Omega_b h^2$ dependence.\(^2\)

\[
\Delta Y_p = +0.4274 \Delta \Omega_b h^2 + 2.043 \times 10^{-4} \Delta \tau_n \\
+1.348 \times 10^{-2} \Delta N_{\text{eff}} - 9.805 \times 10^{-4} \Delta N_{\text{eff}}^2
\] (3.1)

\(^2\)After a typo, 0.39→0.039 in [38], eq. 63, has been corrected.
\[ \frac{\Delta D}{H} = -1.878 \times 10^{-3} \Delta \Omega_b h^2 + 1.256 \times 10^{-8} \Delta \tau_n + 3.564 \times 10^{-6} \Delta N_{\text{eff}}, \]  
\[ \Delta ^{3}\text{He}/H = -2.783 \times 10^{-4} \Delta \Omega_b h^2 + 1.617 \times 10^{-9} \Delta \tau_n + 5.074 \times 10^{-7} \Delta N_{\text{eff}}, \]  
\[ \Delta ^{7}\text{Li}/H = +4.767 \times 10^{-8} \Delta \Omega_b h^2 + 2.4541 \times 10^{-13} \Delta \tau_n - 4.686 \times 10^{-11} \Delta N_{\text{eff}}. \]  

These fits also consider the variations induced by a change in \(-1 < \Delta N_{\text{eff}} < +1\) where \(N_{\text{eff}}\), the effective number of relativistic degrees of freedom, is defined by:

\[ \rho_r = \left[ 1 + \frac{7}{8} N_{\text{eff}} \left( \frac{T_\nu}{T} \right)^4 + \frac{15}{\pi^2 T^4} \rho_\gamma \right] \rho_\gamma. \]  

At recombination, \(\rho_e \ll \rho_r\) and \((T_\nu/T)^4 = (4/11)^4/3\), so that eq. (3.5) matches the definition used in CMB analyses.

4 Method

4.1 Monte Carlo

[15] used a network reduced to the 12 main reactions (13 with the \(^3\text{H}(p,\gamma)^4\text{He}\) that plays a negligible role) for which the rate uncertainties are small compared to all other ones, and sampled the rates within the uncertainty range according to a normal distribution. Here, the extended network includes reaction rates that can be uncertain by a factor of a few orders of magnitude due to the lack of experimental data. Hence, we follow [46] and use a lognormal distribution to cope with these large uncertainty factors together with ensuring that the sampled rates are positive:

\[ f(x) = \frac{1}{\sigma \sqrt{2\pi x}} e^{-\left(\ln x - \mu\right)^2/(2\sigma^2)} \]  

(4.1) (with \(x \equiv N_A\langle\sigma v\rangle\) for short). This is equivalent to assumption that \(\ln(x)\) is Gaussian distributed with expectation value \(\mu\) and variance \(\sigma^2\). For the lognormal distribution, one has:

\[ E[x] = e^{(2\mu+\sigma^2)/2}, \quad V[x] = e^{(2\mu+\sigma^2)} \left[ e^{\sigma^2} - 1 \right]. \]  

(4.2)

As discussed in [46] (see their figure 1), for small \(\sigma\) a lognormal distribution and a normal distribution with the same expectation value and variance are close to each other. Hence, since the uncertainty in the 12 main reaction rates are small, using here a lognormal distribution for those reactions makes no difference with [15] results.

To perform the Monte Carlo calculation, we follow the prescription of [61]. Namely the reaction rates \(x_k \equiv N_A\langle\sigma v\rangle_k\), (with \(k\) being the index of the reaction), are assumed to follow a lognormal distribution:

\[ x_k(T) = \exp(\mu_k(T) + p_k\sigma_k(T)) \]  

(4.3) where \(p_k\) is sampled according to a normal distribution of mean 0 and variance 1 (eq. (22) of [61]). \(\mu_k\) and \(\sigma_k\) determine the location of the distribution and its width which are tabulated as a function of \(T\):

\[ x_{\text{med}} \equiv \exp(\mu) \]  

(4.4) is the median rate and

\[ f \equiv \exp(\sigma) \]  

(4.5)
the uncertainty factor. They are deduced from the evaluation of rate uncertainties. For reactions for which “high” and “low” rates\(^3\) are available,

\[
\mu \equiv \ln \sqrt{x_{\text{low}} \times x_{\text{high}}}
\]

and

\[
\sigma \equiv \ln \sqrt{x_{\text{high}}/x_{\text{low}}}
\]

(see [46]). To avoid erratic numerical behavior, we limit the sampling to values lower than one thousand times the median rate, i.e.,

\[
x < 10^3 x_{\text{med}},
\]

(4.8)
to remain within a range already explored [17].

The Monte Carlo calculation proceeds as follows. For each trial labeled by \(i\), we sample randomly a set of \(\{p_{k;i}\}\) different numbers where \(k\) that runs from 1 to \(N\) (number of reactions) is the index of the reaction. Each one follows independently a Gaussian distribution of mean value 0 and variance 1 and is obtained from a standard random number generator. A BBN calculation is performed with the set of reaction rates \(\{x_{k;i}\}\) obtained from eq. (4.3) that produce the set of isotopic abundances \(\{y_{j;i}\}\) obtained in trial \(i\). Here, \(j=^4\text{He}, ^6\text{Li}, ^7\text{Li}, ^7\text{Be}, ^9\text{Be}, ^{11}\text{B}\) and CNO is the index the corresponding abundances after decays of radioactive isotopes \((^7\text{Be}, ^3\text{H}, ^{11}\text{C}, \ldots)\) or summation of \(A\geq 12\) isotopic abundances (CNO). For further analyses, for each trial, not only the final abundances are stored in a database but also all the \(\{p_{k;i}\}\) values. This allows for correlation studies discussed below.

To obtain the primordial abundances and their uncertainties, as tabulated below, \(\Omega_b h^2\) also is randomly sampled, following a Gaussian distribution according to the CMB deduced data. After 30000 such computations, the calculated distributions of abundances are obtained as displayed in figure 1 for \(^7\text{Li}\). The median primordial abundances and associated 68% confidence intervals are then calculated by taking respectively the 0.5, 0.16 and 0.84 quantiles of the abundance distributions (see figure 5 in [46]).

It has been suspected that traditional sensitivity studies, in which only one reaction is varied while the others are held constant, cannot properly address all the important correlations between rate uncertainties and nucleosynthetic predictions [36]. Searching for such correlations was done by [50] for X-ray bursts (see their figures 7 and 8). They have not found new influential reaction, by examining correlations, as compared to their more traditional sensitivity studies. However, we think that it is worth applying this methods to BBN because the density of the “fabric” of a BBN network (\(d, t\) and \(^3\text{He}\) in addition to the usual \(n, p\) and \(\alpha\)-particles induced reactions) is higher, offering more potential paths. For this purpose, the same Monte Carlo calculation is performed, except that \(\Omega_b h^2\) is fixed, to obtain a data base that can be used to study correlations. The Pearson’s correlation coefficient between isotope \(j\) and reaction \(k\) is, then, calculated as:

\[
C_{j,k} = \frac{1}{N} \sum_{i=1}^{N} \frac{(y_{j;i} p_{k;i} - \bar{y}_j \bar{p}_k)}{\sigma_j \sigma'_k}
\]

(4.9)

\(^3\)In the literature one often find tables of reaction rates with labels such as “high”, “low”, “upper”, “lower” or “recommended”. In most recent works e.g. [24, 35], they have well defined statistical significance. In many older works, e.g. [3] they have no precise definition but we still use eqs. (4.6) and (4.7), for lack of anything better, if this is the only source, to calculate \(\mu\) and \(\sigma\), to be used in the Monte Carlo. (See [46].)
where \( y_{j,i} \) is again the final abundance of isotope \( j \) obtained in trial \( i \) with the set of reaction rates \( \{x_{k,i}\} \) obtained from eq. (4.3) with the set of randomly sampled \( \{p_{k,i}\} \). The correlation coefficients are calculated, with \( y_j \equiv \ln(n_j/n_H) \) for \( j \neq ^4\text{He} \) and \( y_{^4\text{He}} \equiv Y_p \) for the abundances. In eq. (4.9), \( \overline{y} \) and \( \sigma_j \) stand for the mean and standard deviation of \( y_j \) \( [p_k] \). If it were not for the condition (4.8), one would have obviously \( \overline{p} \equiv 0 \) and \( \sigma_k' \equiv 1 \) since the \( p_k \) are sampled according to a normal distribution.

4.2 Reaction rates and uncertainties

In this study, the reaction network and the thermonuclear rates comes from [17]. Namely, it includes 59 nuclides from neutron to \(^{23}\text{Na}\), linked by 391 reactions involving n, p, d, t, \(^3\text{He}\) and \(\alpha\)-particles induced reactions and 33 \(\beta\)-decay processes [5]. Reaction rates were taken primarily from [3, 24, 35, 81] and other evaluations when available. Following their sensitivity study a few reaction rates were re-evaluated by [17]; they are also used here. The complete list of reactions with associated references to the origin of the rates can be found in table 4 of [17] (except for \(^7\text{Be}(n,\alpha)^4\text{He}\) for which we use here the [79] rate instead of the TALYS one in [17]). Since our previous Monte Carlo BBN calculations [15], no change has been made concerning 11 of the 12 main BBN reactions rates. We use those from the evaluation performed by [24] except for \(^1\text{H}(n,\gamma)^2\text{D}\) [2] and \(^3\text{He}(\alpha,\gamma)^7\text{Be}\) [22]. A new experiment [44] have provided new data for the \(\text{D}(d,n)^3\text{He}\) and \(\text{D}(d,n)^3\text{He}\) cross section after the [24] evaluation. Within the BBN energy range, the new data fall exactly on the [24] R-matrix fit (see figure 2 of [19]) that has not yet been updated with this new data.

A recent paper by [54] provides new evaluation of \(^4\text{He}, \, \text{D}, \, ^3\text{He}\) and \(^7\text{Li}\) primordial abundances based on new nuclear data, but comparison with this work is difficult. The new data is extracted by an indirect experimental method (the Trojan Horse Method) that requires theoretical input. We use instead the results of direct measurements that provide the same data at, and even below, BBN energies [24], not affected by screening [77]. Besides,
nothing is said of the origin for rate of the $^{3}$He($\alpha, \gamma$)$^{7}$Be used in their calculations, which is known to be essential for $^{7}$Li prediction, and has been updated by [22].

The only modification of the main rates concerns the weak reactions involved in $n+p$ equilibrium whose rates [25] is determined from the standard theory of the weak interaction but needs to be normalized to the experimental neutron lifetime. The latter has recently been revised by the Particle Data Group from $885.7 \pm 0.8$ s [57], used in [15], to $880.1 \pm 1.1$ s [58]. This significant change is due to the inclusion of the [63] experimental value, now comforted by new analyses (see [58, 80] for more details), that was previously left out of the averaging because of its inconsistency with other data. For this quantity, we use the latest value recommended by the Particle Data Group $\tau_n = 880.1 \pm 1.1$ s [58], but are aware that this remains an open debate [80] but that affects essentially, only $^{4}$He.

The calculation of $^{6}$Li/H depends directly on the D($\alpha, \gamma$)$^{6}$Li reaction rate that was plagued with by large uncertainty [3]. New measurement of the D($\alpha, \gamma$) $^{6}$Li which is the main way to produce primordial $^{6}$Li have been performed. In the absence of direct measurements at BBN energy, [32] used the Coulomb breakup technique to extract the cross section. Very recently, a direct measurement has been performed at LUNA [1]. The results of this very difficult experiment agree well with those from the indirect method [32]. So, this confirmed low cross section comforts the prediction of the BBN calculations of a low primordial $^{6}$Li value, $^{6}$Li/H = $10^{-14}$.

For the remaining of the 391 reactions, we use tabulated $\mu$ and $\sigma$ [35], tabulated limits [3, 17, 24, 81] together with eqs. (4.6) and (4.7) and for the others, tabulated rates together with estimated uncertainty factors and eqs. (4.4) and (4.5). In particular, in the work of [17], many rates come from theory (TALYS code) [31] and have not been re-evaluated since then. The TALYS code is obviously not well adapted to this low mass region where level densities are too low to justify the Hauser-Feshbach approach. However, due to the lack of experimental data it can be used as a first guess for the hundred of reaction rates that are needed. To estimate the uncertainty associated with TALYS rates in the relevant ranges of masses and temperature, [17] compared them with experimentally determined reaction rates [3, 35] and found that the differences do not exceed three orders of magnitude at BBN temperatures (see figures 1–11 and 16–21 in [17]). In their sensitivity study, they were not found to influence significantly the results, when individually multiplied by factors up to $10^{+3}$, except for ten reactions whose rates were re-evaluated. Hence, for the rates, labeled “TALYS” in table 4 of [17], we use here uncertainty factors of $f=100$ (i.e. $\sigma = \ln(100)$). (Those, labeled “TALYS” in bold face in the same table were re-evaluated so that calculated uncertainties are available.) For rates provided without calculated uncertainty, labeled e.g. “CF88”, “MF89”, “Wag69”, . . . , (see refs. in [17]) we generally adopted $f=3$, except when the uncertainty is not provided but is obviously smaller e.g. “Ham10” [32] or “Nag06” where we adopted a 40% uncertainty ($f=1.4$). This may look arbitrary, but one of the main goal of this work is to identify potentially influential reaction rates that may have to be improved in a subsequent stage.

5 Results concerning $^{4}$He, D, $^{3}$He and $^{7}$Li

Figure 2 displays the $^{4}$He, D, $^{3}$He and $^{7}$Li abundances calculated as a function of $\eta$ by Monte Carlo with the full network, and evaluated rate uncertainties following [17], compared to our previous work with a reduced network [15]. At $\eta_{\rm CMB}$, the differences are hardly visible except for $^{4}$He, due to the updated neutron lifetime. Comparison between columns 2 and 5
Figure 2. (Color online) $^4$He, D, $^3$He and $^7$Li abundances as a function of $\eta$ calculated by Monte Carlo with the updated full network (dark blue) or with the reduced network as in ref. [15] (light blue dashed). The vertical areas correspond i) to the WMAP (dot, black) and ii) Planck (solid, yellow) baryonic densities. The horizontal areas (hatched green) represent the adopted observational abundances while the horizontal dotted lines correspond to those previously used [7, 49]. The (red) dash-dotted lines correspond to $Y_p$ calculated with $N_{\text{eff}} = 3.30 \pm 0.27$ derived from the CMB [55].
in table 1 shows the evolution of the yields from [15] with the first WMAP results [64] to the recent Planck data [55]. The reduced uncertainty on D/H is a direct consequence of the reduced uncertainty on $\Omega_b h^2$ while $^7$Li uncertainty is still dominated by nuclear uncertainty on the $^3$He($\alpha,\gamma$)$^7$Be rate.

Figure 2 displays the abundances as a function of $\eta$ and table 5 those at the Planck baryonic density, both for $N_{\text{eff}} = 3$, as defined by eq. (5.5). When using the last evaluation of $Y_p$ [8] deduced from observations, we obtain $2.19 \leq N_{\text{eff}} \leq 3.63$ at Planck baryonic density. This interval is given after corrections to the weak rates [25, 47, 48] have been introduced as discussed in section 3. It includes the correction for non-instantaneous neutrino decoupling in the presence of oscillations, introduced as a constant shift $\Delta Y_p = +0.0002$ [48] instead of a slight increase of $N_{\text{eff}} = 3$ since, if this approximation works for $^4$He, the change for the other nuclides is exactly in the opposite direction of the true one (see [48] for details). In figure 2 we also display for visual inspection the results obtained for the limits on effective number of neutrino family $N_{\text{eff}} = 3.30 \pm 0.27$ derived from the CMB only confidence interval [55].

Finally in table 5, a comparison between this work and the last observational data is proposed: an overall consistency between standard BBN calculation and the observational constraints is presented except for lithium, as explained above: the discrepancy remains of the order of 3.

### 6 Results concerning $^6$Li, $^9$Be, B, C

Figure 3 displays the $^6$Li, $^9$Be, $^{10}$B, $^{11}$B and CNO abundances calculated as a function of $\eta$ including our estimated uncertainties from the Monte Carlo, and a comparison with observations. The displayed uncertainties are obtained by calculating for each value of $\eta$, the 0.16 and 0.84 quantile [46] of the distributions. The corresponding confidence intervals at $\eta_{\text{CMB}}$ are displayed in table 4 and are orders of magnitude below observations (section 2.2).

Figure 4 displays the histogram of CNO/H obtained from our Monte Carlo calculation, from which it is possible to extract the 0.16, 0.5 and 0.84 quantile, respectively given by
Figure 3. Standard big bang Nucleosynthesis predictions for the abundances of $^6\text{Li}$, Be, B and CNO isotopes as a function of baryonic density, compared to some observations. The horizontal lines and areas correspond to the $^6\text{Li}$ observation in HD 84937 (green), beryllium (magenta) and boron (light blue) upper limits, and CNO lower limit to affect Population III stars; see text.
Figure 4. CNO/H distribution showing that high values are obtained in a non negligible proportion.

4.94×10^{−16}, 9.63×10^{−16} and 2.85×10^{−15}. This is very close to the range CNO/H = (0.5−3.) × 10^{−15} estimated by [16] from the results of [17]. However, at high value, the tail of the distribution (≈3%) extends to values much above the CNO/H = 10^{−13} limit. At first, it seems straightforward to extract the subset of events, for which e.g. CNO/H > 10^{−13}, and examine the corresponding sampled reaction rates (i.e. the p_k’s in eq. (4.3)) that are stored together with the final abundances in a database. However, since all ≈400 p_k’s are different from one trial to the other, it was not possible to identify combination of reaction rates that produced such an effect. To identify those combinations of reaction rates that allows such high value, we relied upon the calculated correlations between rates and yields.

This method is complementary to the one used by [17], in which a single reaction was tested at a time by changing its rate by factors of 10^n, n = −3, −2, −1, 1, 2, 3. Here all rates are simultaneously changed by factors, different for each reaction, and randomly sampled as described above. This allows to identify sub-networks rather than individual reactions and takes into account the different uncertainty factors. Results are displayed in tables 5–12 when their absolute value exceed 10%. Note however that a higher sensitivity, as calculated in [15, 17], does not necessarily correspond to a higher correlation as calculated here. Our previous sensitivity studies assumed an arbitrary ±15% rate variation [15] or a factor of up to 1000 rate variation [17]. Here, while, when sampling the rates, we still allow for large arbitrary rate variations for reactions with no documented rate uncertainties, we restrict the variations to evaluated rates and associated uncertainties when available. These latter reactions include e.g. those evaluated by [24] or those identified as influential in a first step, but evaluated in a second step by [17]. For instance, the most influential rate on 7Li+7Be is 1H(n,γ)2H [15] but its rate uncertainty is very small [2] so that it does not appear in the table, contrary to the next most influential, 3He(α,γ)7Be whose rate uncertainty is still not negligible and thus appears in table 8.

We use this simple criterium but are aware that more sophisticated criteria need to be developed: see e.g. figure 6 in [36].
The reactions that appear most correlated with the isotopes lighter than C (tables 5–11) are among those found in previous studies. In table 12, it appears that besides the already known influential reactions on CNO production [17] [7Li(d,n)2He, 12B(p,α)10Be, 8Li(α,n)11B, 13C(d,α)11B], new influential reactions are found. It indicates a new possible path for CNO production involving 10Be, namely: 10Be(p,α)7Li, 10Be(α,n)13C, 7Li(t,γ)10Be, 8Li(t,n)10Be, 10Be(t,n)12B and 10Be(p,t)24He. Note that all these new reactions involve radioactive isotope(s) [6H, 9Li and 10Be] in the initial state, hence the absence of direct experimental data. From this analysis, it is obvious that a new chain of reactions leading to CNO via 10Be need further attention as it could, depending on the cross-sections, provide a more efficient source of CNO.

These reactions were not identified in our previous work [17], because we varied the rates, one at a time, (by factors of $10^n$ with $n$ varying from −3 to 3 by steps of one unit). For instance, when increasing the 8Li(t,n)10Be or 10Be(α,n)13C rates by a factor of 1000, the CNO abundance only increase by 30% [17] while if both rates are increased by the same factor, CNO/H is found to be higher by a factor of 200. This is the purpose of the following analysis to identify such potential new paths. Hence, we first allowed all rates to vary simultaneously and independently according to lognormal distributions. Now, to better identify the chains of reactions that may lead to an increased CNO production, we allow the rates of the 6 newly identified reactions listed above to vary within a few orders of magnitude as in ref. [17] but considering all possible combinations. We chose factors of $10^{±2}$ variations on rates w.r.t. TALYS calculated rates which are consistent with our comparison between TALYS and experimentally measured rates [17] and select those combinations of factors that leads to a CNO/H production higher than $10^{-13}$, the minimum value to affect Pop III stars [27]. In table 13 are displayed the 9 combinations (out of 3^9 = 729 combinations ) of signs in the exponent of the $10^{±2}$ factors (with “0” meaning no rate variation) for which CNO/H > $10^{-13}$. (Obviously, we could have reduced the number of combinations: taking higher/lower rates for production/ destruction of 10Be but we found it was not worth the trouble.) Table 13, shows that the 7Li(t,γ)10Be and 10Be(t,n)12B reactions are not essential since whatever the exponent (-2, 0 or +2) of the variation factor, the result is not significantly affected. On the contrary, the combination of higher rates for 10Be(α,n)13C and 8Li(t,n)10Be together with lower rates for 10Be(p,α)7Li and 10Be(p,t)24He result in a substantial increase in primordial CNO production. From this combinatorial analysis we could, hence, separate within the set of 6 reaction rates that were weakly correlated to CNO/H those 4 that really matter. The factors of $10^{±2}$ variation w.r.t. TALYS rates is conservative (see section 4.2) so that even higher CNO yields can be expected. Experimental investigations of these four reactions (figure 5) are hence highly recommended.

Afterwards, the production of this short list of reactions involving 10Be for the production of CNO may seems straightforward but dealing with a relatively large and dense network (i.e. including p, n, α, d, t and 3He induced reactions) is not so easy. First, among all the reaction paths that could connect A < 8 to CNO nuclei, the study of correlations allowed us first to identify, the six reactions of table 13 that did not show up in our (or any other) simpler sensitivity analysis [17] of the same network. Second, the extensive combinatorial analysis allowed us to finally select out four reactions.

This work has updated the BBN predictions in order to take into account the most recent developments concerning the cosmological framework (i.e. the cosmological parameters determined from the recent CMB Planck experiment). It demonstrates that these predictions are robust for the lightest elements. It shows also that the modification of these parameters in
the range allowed cannot alleviate the lithium problem; concerning primordial CNO production we show that higher CNO yields can be expected: the four reaction rates $^{10}\text{Be}(\alpha,n)^{13}\text{C}$, $8\text{Li}(t,n)^{10}\text{Be}$, $^{10}\text{Be}(p,\alpha)^7\text{Li}$ and $^{10}\text{Be}(p,t)^{2}\text{He}$, could be investigated to test this result.

Finally, we want to emphasize the use of statistical methods in BBN have lead to the identification of a possible new path to CNO. For this, we have used the simple Pearson’s correlation coefficient to discriminate important reactions. This is obviously a first step: more elaborate statistical techniques could be developed and also applied to other nucleosynthesis sites [36].
Table 13. Each column correspond to a combination of multiplicative factors ("-" for $10^{-2}$, "0" for $10^0$ and "+" for $10^+2$) which applied simultaneously to all the six TALYS reaction rates lead to CNO/H > $10^{-13}$.

![Diagram of BBN nuclear network with in red the new possible paths to CNO.](color online)
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A Relation between $\eta$ and $\Omega_b h^2$

Here, for precise comparison with other works that quote $\eta$ numerical values rather than $\Omega_b h^2$ ones, we recall here the numerical relationship between the two. This was calculated previously by [69]; here we detail our own calculation.

What is important for BBN is the baryonic density $\rho_0,\rho_{0,c}$ where $\rho_{0,c}$ is the present day critical density given by (numerical values of physical constants are taken from [58], atomic masses from [78]):

$$\rho_{0,c} = \frac{3H_0^2}{8\pi G} = 1.87847 \times 10^{-29} \text{ g/cm}^3,$$  \hfill (A.1)

that allows for the calculation of

$$\rho_b(t) = \left[1.87847 \times 10^{-29} \text{ g/cm}^3\right] \times \Omega_b h^2 a^{-3}(t),$$  \hfill (A.2)

to be used in the network calculations. The photon density (number/cm$^3$; $T_0 = 2.7255$ K; $\zeta(3) = 1.20206$) is:

$$n_\gamma(T) = \frac{2\zeta(3)}{\pi^2} \left(\frac{k_B T}{\hbar c}\right)^3 = 410.73 \left(\frac{T}{T_0}\right)^3 \text{ cm}^{-3}$$  \hfill (A.3)

The number of baryon per photon is thus given by:

$$\eta = \frac{\rho_{0,b}}{n_\gamma(T_0)M} = \frac{3H_0^2}{8\pi G \zeta(3)} \left(\frac{\hbar c}{k_B T_0}\right)^3 \left(M_p(1 - Y_p) + \frac{M_\alpha}{4} Y_p\right)^{-1} \Omega_b$$  \hfill (A.4)

where $M$ is the mean baryon mass

$$M = M_p(1 - Y_p) + \frac{M_\alpha}{4} Y_p = (1.6735 - 0.0119 Y_p) \times 10^{-24} \text{ (g)}.$$  \hfill (A.5)

So that the relation between $\eta$ and $\Omega_b h^2$ are:

$$\eta = 2.7381 \times 10^{-8} \Omega_b h^2 \text{ or } \Omega_b h^2 = 3.6521 \times 10^7 \eta$$  \hfill (A.6)

for $Y_p=0.27$ (solar, $M = 1.6703 \times 10^{-24}$ g) or

$$\eta = 2.7377 \times 10^{-8} \Omega_b h^2 \text{ or } \Omega_b h^2 = 3.6528 \times 10^7 \eta$$  \hfill (A.7)

for $Y_p=0.246$ (BBN, $M = 1.6706 \times 10^{-24}$ g). When using the same values for $T_0$ (2.725 instead of 2.7255 K here) and $Y_p$ (0.27), our result differs by less than 0.004% from the [69] one. The uncertainty on the present day CMB temperature ($T_0 = 2.7255 \pm 0.0006$ [58]) induces an uncertainty of less than 0.07% on the calculated coefficient.
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