Carbon in the pregalactic epoch and the search for the first haloes

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ABSTRACT

A possible way of detecting first structure formation in a non-standard BBN Universe during the dark age, due to resonant scattering of the CMBR photons in the rotational lines of the primordial CH molecule is discussed. The calculations are made within the framework of the ΛCDM cosmology and plausible first structure physical conditions. The carbon chemistry during the pregalactic epoch is considered. The relative abundance of the CH molecule is found to be 10(-14) whereas the adopted \([C]/[H]\) ratio was taken to be 10(-10). The optical depth, \(dT/T\) and integration times are estimated. The calculated optical depth turns out to have high values, that argue in favor of this molecule as an excellent candidate in searches for first structure formation. Possible observations with the GMT and ALMA are discussed.

Key words: cosmology: first stars, galaxies: formation, molecular processes

1 INTRODUCTION

The investigation of the epoch of first structure formation in the early Universe is one of the most intriguing aspects of modern cosmology. The observational data on the physical conditions during the growth of the first structures, if detected, would give us extremely important information on the fundamental problems of the early Universe, such as inflation, Big Bang Nucleosynthesis (BBN) models (see for example the review by Steigman (2006) and references therein), the formation of the first mini-galaxies (see Yoshida et al. (2003); for a review, as well as [Mashchenko et al. (2006) and reference therein], first miniquasars (Kuhlen & Madau (2003)) and PopH\(\star\) stars (O’Shea & Norman (2007); Vasiliev & Shchekinov (2003; Yoshida et al. (2006)). As has been discussed in previous works, the most promising way to investigate this epoch, is to search for the Spectral Spatial Fluctuations (SSF), produced by the primordial molecules in the spectra of the CMBR through resonant scattering of the CMBR photons. Recently, the possibility of detecting these lines with ODIN and Herschel satellites has been investigated by Maoli et al. (2005). They have also discussed the current observational situation for molecules based on the light elements. For further details, see Maoli et al. (1996), and the most recent calculations of the SSF due to the HD molecule in Núñez-López et al. (2006). It must be stressed here that in the case of deviation from the simple equilibrium evolution of the Universe, the abundance of light elements in some regions of the Universe can increase (see for example possible production of deuterium by cascades from energetic antiprotons considered in the paper of Levitan et al. (1988)), that can lead to the observability of such regions.

The SSF from molecules based on the light elements (such as \(H, D, He, Li\)) in the primordial gas has been discussed by many authors during the last decade. But, perhaps light elements are not the only species capable of leaving footprints in radio. In recent years, models of Non-standard Big Bang Nucleosynthesis (NBBN) and new physics have attracted considerable attention, motivated in part for the discrepancies that remain between the abundance measurements of \(^4He\) and \(^2H\) (Steigman (2006)). The NBBN models predict a wide range of abundance for the heavy elements, which could be used to discriminate, combined with future observational results, among the alternative models. In this regard, and for reasons that will be discussed in this paper, the abundance of primordial carbon appears to be of particular interest. One obvious reason, is related to the peak in abundance for the \(C-N-O\) group, whose height has a strong dependence on the NBBN model. In particular, the \(^{12}C\) relative abundance can vary from \(3 \cdot 10^{-14}\) for the standard BBN (see for example Lara (1998)), up to \(10^{-9}\) (Rauscher et al. 1998). Recently the model of Inhomogeneous BBN has been revisited by Lara et al. (2006), where the relative abundance of \(^{12}C\) has been found to be of the order of \(10^{-12}\) (Lara 2007). Besides, the Nonequilibrium Cosmological Nucleosynthesis discussed in the papers

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of Khlopov et al. (1994) and Sedel’nikov et al. (1993) can still further increase its abundance.

The chemistry of the early Universe has also been a subject of investigation in the last few years. For a review on this topic one may read Galli & Palla (1998) and more recently, the results for the deuteron chemistry in Galli & Palla (2002). But little effort has been done so far to consider the assumption of the NBBN, for which, the chemistry of heavy elements has to be included.

Recently, the chemistry of the primordial carbon and oxygen in the early Universe was calculated (Lipovka et al. 2002a) and the possibility of direct observations of the CH molecules formed in the first halos was discussed (Lipovka et al. 2002b; Campos et al. 2006). It needs to be stressed that not just primordial carbon should be taken into consideration, but also carbon produced by primeval SN. First stars (PopIII) possibly appear at \( Z \approx 20 \), and must significantly enrich the environment with heavy elements. For example, Daigne et al. (2004), consider a model in which the relative abundance of \(^{12}\text{C} \) at \( Z = 19 \) due to feedback can reach a value of \( [\text{C}]/[\text{H}] = 10^{-4} \).

It should also be noted, that the formation epoch of the first stars can be pushed back to even higher redshifts due to the presence of ultra-high-energy cosmic rays which stimulated the formation of the first stellar objects, as it has been recently suggested by Vasiliev & Shchekinov (2006). If this is the case, one can consider significant abundance of carbon at very early epochs.

It is for these reasons, that the search for primordial carbon is of special interest. On the one hand, the detection of primordial CH would help us discriminate among the NBBN models. On the other, it would allow us to obtain important information about the formation of first structures in the Universe (such as minigalaxies, first stars, etc.).

The \( \text{CH} \) molecule is an excellent species for this aim due to several reasons:

1) \(^{12}\text{C} \) is rather sensitive to the NBBN model.

2) It is argued here that \( C \) stands a better chance for primordial chemistry than the other two species in the \( C NO \) abundance peak of the BBN element distribution. Although \( N \) has an abundance a little bit higher than \( C \), its negative ion \( N^- \) has a binding energy an order of magnitude lower than that of \( C^- \), and the ratios for \( NH \) molecule formation are quite low. With respect to oxygen, its relative abundance is much lower compared with that of \( C \) (see Lipovka et al. (1998)) and the molecules based on primordial oxygen are less interesting than those of \( \text{CH} \) (see also Lipovka et al. (2002a)).

3) \( \text{CH} \) has a rather high dissociation energy (3.46 eV) and a large dipole moment.

4) Because of the rather low densities in the cosmological gas there is no depletion chain \( C-\text{CH} \rightarrow \text{CH}_2-\text{CH}_3 \rightarrow \text{CH}_4 \), like the one that exists in the interstellar medium. For this reason, the kinetics of the ISM is significantly different to the cosmological one.

Several facilities being planned or under construction will cover the submillimeter and millimeter wavelength ranges with high sensitivity. Examples of these are ALMA, CARMA, and the Large Millimeter Telescope (LMT), under construction in Mexico, whose radiometers will cover the range from 0.8 to 3 mm. The redshifted rotational lines of the primordial CH molecule are expected to fall in the mm region, and the optical depths for first structures are estimated to be rather high. The feasibility of detecting CH in the near future, is one of the main motivations for doing detailed calculations for this molecule.

The aim of the present work is to draw attention to the problem of heavy elements in the early Universe, and to emphasize on the extremely important role primordial carbon can play in the investigation of the galactic epoch, as well as in the BBN models. Here we present for the first time, the complete chemistry of primordial carbon and calculate the expected footprints of first structure under formation in the rotational lines of the CH molecule on the basis of the \( \Lambda \) - Cold Dark Matter (\( \Lambda \) CDM) scenario of cosmic structure formation.

The paper is organized as follows: in the second section we present the chemistry of primordial carbon in the early universe. In the third, the observational parameters for first halos in the dark age epoch are introduced. Finally, the main conclusions are discussed in the fourth section.

### 2 CHEMISTRY OF PRIMORDIAL CARBON

The chemistry of the light elements under the standard BBN model has been discussed in several papers (see for instance, the review paper Galli & Palla (1998) and will not be discussed in any detail here. Recently the chemistry of fluorine in the early Universe was investigated by Puy et al. (2007) (see also references therein for the standard light element chemistry).

The chemistry of the primordial carbon and oxygen in the early Universe was considered for the first time in Lipovka et al. (2002a). In the present work the primordial carbon chemistry is revisited to make it more complete and up-to-date with more recent data for the molecular processes. Within the framework of the \( \Lambda \) CDM Universe, the parameters adopted for the calculations are as follows: \( \Omega_m = 0.27 \), \( \Omega_b = 0.04 \), \( \Omega_{\Lambda} = 0.73 \) and \( H_0 = 71 \) km s\(^{-1}\)Mpc\(^{-1}\). (e.g., Spergel et al. (2003)). Standard BBN yields of the light elements are assumed for simplicity, since their deviation from the standard values do not significantly affect the carbon chemistry. The kinetic equation of the system written in terms of the redshift \( z \) is given by the following expression:

\[
dx_i \ \frac{dx}{dz} = \frac{1}{H_0 (1 + z) \sqrt{\Omega_m (1 + z)^3 + \Omega_{\Lambda}}} \times \left[ n_0 (1 + z)^3 \left( \sum_{k,j} x_k x_i R_{kji} - x_i \sum_{m,n} x_m R_{imn} \right) + \sum_k x_k R_{kij} - x_i \sum_m R_{im} \right],
\]

where \( dz = dtH_0 (1 + z) \sqrt{\Omega_m (1 + z)^3 + \Omega_{\Lambda}} \), \( n_0 \) is the density of the gas in the present epoch, \( x_i \) are the dimensionless relative abundance for the \( i \) species (\( x_i = n_i/n_{tot} \)), \( R_{ijk} \) are the rates of the collisional processes \( i \rightarrow j \rightarrow k \), as functions of the kinetic temperature \( T_k \), \( R_{ij} \) are the rates of the radiative processes (formation and destruction of the molecules by the CMBR photons characterized by the
radiative temperature $T_r$). To calculate the kinetic temperature $T_r$, we need to solve the following equation:

$$\frac{dT_r}{dt} = -2T_r H_0 \sqrt{\Omega_M (1 + z)^3 + \Omega_k + \frac{2 (\Gamma_{mol} - \Lambda_{mol})}{3nK} + \frac{\Theta_{th}}{3nK} + \frac{2T_r}{3n} \left( \frac{dn}{dt} \right)_e + \frac{8\pi a_b T_r^4}{3m_e c} x_e (T_r - T_c).} \quad (2)$$

Here, the first right-hand term is for the Hubble expansion of the Universe, the second one corresponds to heating (\( \Gamma_{mol} \)), or cooling (\( \Lambda_{mol} \)) of the gas by absorption or emission, the third term describes the heating (cooling) of the medium in exothermic (endothermic) chemical reactions, the forth one appears here to take into account the change of the primordial gas density due to chemical reactions, which approximately corresponds to redshift $Z=500$. For this reason, we need to calculate this rate coefficient for a wider range of temperatures, from $T_k = 100K$ to $3000K$. We have calculated this rate coefficient in our paper (Campos et al. 2007) by using the principle of detailed balance and cross section for the inverse process - photodetachment (see above), as suggested by Moskvin (1964). In this way, we obtain a rate coefficient which has the correct behavior with the kinetic temperature (approximately constant), like those for the hydrogen radiative attachment ($H + e^- = H^- + \gamma$). It can be approximately described by the following expression:

$$R_{rad} = 1.53 \cdot 10^{-15} \left( \frac{T_r}{300} \right)^{-0.01} \text{[cm}^2 \text{s}^{-1}], \quad (6)$$

which has been adopted in our model.

### 2.3 Associative detachment

There are two process of associative detachment of interest. The first one is

$$C^- + H = CH + e^-,$$

and the second is

$$H^- + C = CH + e^-.$$

These were adopted in our calculations with the rate constant $5 \cdot 10^{-10}$ and $10^{-9} \text{[cm}^3 \text{s}^{-1}]$ respectively from the UMIST data base.

### 2.4 Other important reactions

Besides those mentioned above, we revisited and incorporated another process which was not taken into account in our previous calculation (Lipovka et al. 2002a). As it was mentioned in that paper, the main channel for the CH molecule formation (destruction) are the neutral-neutral reactions $C(H_2, H)CH$ and $CH(H, H_2)C$. The most recent review and data on these processes was presented by van Harrevelt et al. (2002) (see also references therein).

As discussed by Lipovka et al. (2002a) one of the most important channels for the CH molecule formation, is the $C + H_2 = CH + H$ reaction. It was investigated in detail in (Guadagnini & Schatz 1996), where the cross section for this process was proposed, and reported to be in excellent agreement with the experimental data. The rate coefficient for this reaction is given by the following expression

$$R_1 = 1.16 \cdot 10^{-9} \left( \frac{T_r}{300} \right)^{0.5} \exp \left( \frac{-14100}{T_r} \right) \text{[cm}^3 \text{s}^{-1}], \quad (9)$$

The inverse process $CH + H = C + H_2$ is the main
The calculations of the molecular abundance were carried out for a temperature of 300K, and for these reasons it was expected to be higher, and so the chemistry must be faster. Moreover, the calculations were made neglecting deuterium and lithium, their small abundance. In our calculations we use the hydrogen and helium abundance according to the Standard BBN and did not take into consideration deuterium and helium, due to their insignificant role in the CH molecule production. We include helium because of the importance of the $He^+$ molecular ion in the production of $H_2$ by the chain of reactions $HeH^+ + H = H_2 + He$; $H_2 + H = H^+ + H_2$. The BBN carbon abundance was adopted from the paper of Rauscher et al. (1994) to be equal $[C]/[H] = 10^{-9}$. It is an estimation which can easily be changed to other abundance ratios, because it appears linearly in the equations.

The results of the calculation are shown in Fig. 1 for the range of redshift from $z = 400$ and up to $z = 10$. The relative abundance of the CH molecule is shown by a solid line and in this way it is possible choose a more convenient scale to see the curves for $CH_3$, $C^+$, $CH^+$, $CH_2^+$, $CH_3^+$, and $C^-$.

3 OPTICAL DEPTH AND OBSERVATIONAL ESTIMATES

It is well known that the largest resonant line opacities in homogeneous mass perturbations are produced when they are at their maximum expansion or turn-around epoch (linear stage of their evolution), when all parts of the protocloud participate in the line formation process.

Let us estimate the detectability of line features of the primordial CH molecule in protostuctures still in their linear or about-linear evolution regime, i.e. before gravitational collapse and first star formation occurs. Here we calculate the CH resonant line opacities only at the turnaround epoch for CDM high-density $(6 - \sigma)$ mass perturbations. The interaction of CMBR photons with the primordial molecules inside these protostuctures will produce spectral - spatial signatures in the CMBR spectrum, containing information on the physical conditions of the gas prior to the formation of the first stars and minigalaxies in the universe.

The optical depths of primordial protoclouds in the rotational lines of CH molecule were calculated using the spherical top-hat approach (see for example Padmanabhan 1993; Tegmark et al. 1997), to obtain the epoch, density, and size of the CDM mass perturbations at their maximum expansion, for the $\Lambda$CDM cosmology. We have discussed the top-hat approach in our previous paper (see Núñez-López et al. 2006), and the parameters of the first structures listed in Table 1 and Table 2 of that paper will be used here. Table 2, in particular, presents the parameters we need for 6σ halos such as the turn-around redshift, size of protoclouds, density etc.
The optical depth for a protocloud of size $L$ is given by:

$$\tau_\nu(L) = \int_0^L \alpha_\nu \, dx,$$  \hspace{1cm} (11)

where the integration is carried out over the line of sight and $\alpha_\nu(x)$ is the absorption coefficient given by the following expression:

$$\alpha_\nu = \frac{\lambda^3 (2J' + 1)}{8\pi (2J + 1) V_T} x_{CH n_J n_{tot}} A_{J'J} \left(1 - e^{-\tau_\nu}\right).$$  \hspace{1cm} (12)

Here $\lambda$ is the wavelength, $J$ is the rotational quantum number, $x_{CH}$ is the relative abundance of the CH molecule shown in fig. 1, $n_J$ is the population of $J$-th rotational level at epoch $z$, and $A_{J'J}$ is the Einstein coefficient.

By using these expressions, we calculate the CH line optical depths corresponding to protoclouds of several masses at their turnaround redshifts. The result is shown in Fig. 2 for three ground rotational line transitions $3/2(2 \Pi_{1/2}) - 1/2(2 \Pi_{1/2})$, $5/2(2 \Pi_{1/2}) - 3/2(2 \Pi_{1/2})$, and $3/2(2 \Pi_{1/2}) - 1/2(2 \Pi_{1/2})$ for the 6$^*$ first halos.

As we can see, the values of the optical depth for the CH molecule lines are much larger than those reported for the HD molecule (Núñez-López et al. 2006) and reach values $10^{-4}$ for redshift $z = 20$.

Let us now estimate some observational parameters for the first structures in the CH rotational lines. The temperature fluctuations of the CMBR due to the resonance scattering of the CMBR photons by moving protoclouds is:

$$\frac{\Delta T}{T} = \frac{V_p}{c} \tau.$$  \hspace{1cm} (13)

Here $V_p = V_p(z)$ is the peculiar velocity of the protocloud at epoch $z$ with respect to the CMBR, $c$ is the speed of light, and $\tau$ is the corresponding optical depth of the protocloud at epoch $z_{tu}$.

The linear theory of gravitational instability shows that the peculiar velocity of every mass element grows with the expansion factor $V_p(z) \propto \dot{D}(z)/(1 + z)$. An accurate approximation to this expression for a flat universe with a cosmological constant is suggested in the papers (Lahav 1991) and (Carroll et al. 1992). The value of the peculiar velocity at the present epoch $V_p(0) \approx 650$ km/s, adopted in our calculation, was taken from (Lauer & Potsman 1994), (Hudson et al. 1999, 2004), and (Willick 1999). By using this expression and the CH optical depths shown at Fig. 2, one can estimate with eq. (13) the temperature fluctuation of the CMBR secondary anisotropies. In our case for the redshift $z = 20$, for the case of the 6$^*$ protohalos, we obtain $\Delta T/T \approx 2 \cdot 10^{-7}$ in the 5/2 3/2 rotational transition at the laboratory wavelength $\lambda_0 = 181 \mu m$, whereas for the case of collapsed halos this value can be higher.

Let us now estimate the integration time required for the detection of the secondary anisotropies with modern telescopes (such as ALMA, CARMA or LMT/GTM). The observational time $\Delta t$ can be estimated from the equation

$$\Delta T = \frac{T_0}{\sqrt{\Delta \nu \Delta t}}.$$  \hspace{1cm} (14)

where $\Delta \nu$ is the bandwidth, $T_0$ is the noise temperature and $\Delta t$ is the amplitude of the temperature fluctuations calculated above. For $\Delta \nu$ we adopt an estimation $\Delta \nu \approx 0.1$ and $T_0 \approx 50$ K. Thus, for the 6$^*$ protohalos, the integration time required for an observable signal of the rotational transitions of CH molecules is estimated to be $\Delta t \approx 7 \cdot 10^7$ s = 200 hours, which can be divided into 10 - 20 sets of observations near the north (south) pole regions. It should be stressed here that for the case of collapsed gas inside virialized $3\sigma$ halos, previous to star formation triggering (see for detail the discussion in Núñez-López et al. 2006), the integration time needed for the detection of the rotational lines of the primordial CH molecule, can be reduced to up to a few hours.

To conclude this part, the angular size of the objects must be mentioned. The first halos discussed in the present paper are actually the same considered in our previous paper (Núñez-López et al. 2006), for which the signatures of the HD primordial molecule were investigated. For this reason we do not need any special consideration here and can refer to Fig. 3 in that paper. It should be noted that the angular size for all protoclouds reaching their maximum expansion in the redshift range of $20 < z < 40$ (which corresponds roughly to a mass range of $10^5 M/\odot < 10^6$ and $10^6 M/\odot < 10^{11}$ for the $3\sigma$ and $6\sigma$ cases, respectively) appears within the observable region of ALMA and CARMA.

4 CONCLUSIONS

In the present paper we present for the first time the calculations of the kinetics of the primordial CH molecule and the observational estimates for protoclouds during the first structure formation epoch, which can possibly be observed in the CH molecule rotational lines. The signature of the first structure formation epoch is actually the Spectral-Spatial Fluctuations in the CMBR spectrum due to the elastic resonant scattering of the CMBR by primordial CH molecules in its rotational structure. The optical depths in the pure
rotational structure of the molecule were calculated for the 6σ halos within the framework of a ΛCDM universe.

For our calculation, we adopt the relative abundance of primordial carbon \([C]/[H] = 10^{-3}\) taken from the paper of Rauscher et al. (1994). By taking into account the fact that the relative abundance of the CH primordial molecule depends linearly on the \([C]/[H]\) value, one can easily reestimate the results for any particular case of NBBN. The main results of this work can be summarized as follows:

1) We calculate for the first time the chemistry of primordial carbon in the case of Nonstandard BBN. This was done for an homogeneous primordial gas.

2) It is shown that the most abundant of the carbon-bearing molecules is CH, whereas others (such as \(CH_2, CH_3, CH_5, CH_7, CH_9, CH_{11}, CH_{13}, CH_{15}, CH_{17}, H_2C, C_2H, C_2H_2, C_2H_4, C_3H_2, C_3H_4\)) only appear in negligible amounts. This difference, if compared with the interstellar medium, can be explained in terms of the rather low abundance of primordial gas and carbon. It must be stressed that in the presence of inhomogeneities, the CH molecule abundance increases, so that in this sense, these calculations can be considered as lower limit estimations.

3) Within the framework of the ΛCDM universe we calculate the optical depth for pure rotational lines of the primordial CH molecule for first structures formed during the Dark Age epoch. At redshifts \(z = 20\), for the 6σ model, the calculated optical depth is \(\tau_{\text{opt}} \approx 10^{-4}\), in two ground and one exited rotational transitions. The frequencies of observation for these three lines are \(\nu \approx 25, 80, 96\, \text{GHz}\) that correspond respectively, to the redshifted lines of the rotational transitions \((J,K) = (3/2 - 1/2); (5/2 - 3/2); (3/2 - 1/2)\) of the CH molecule (see Fig. 2). We would like to stress here, that the presence of tree observable lines with not too different optical depths, would permit to identify the observed object as a first halo with a redshift \(20 - 30\).

4) For testing NBBN models, the CH molecule is a more efficient tool in searches for signatures of the first structure formation epoch than the HD molecule, discussed in our previous paper (Núñez-López et al. 2006). Furthermore, the CH rotational lines (even if not detected) would allow us to discriminate between the NBBN models. The optical depth of first halos in rotational lines of CH in the case of NBBN model discussed in the paper of Rauscher et al. (1994), is larger than that for HD by a factor of \(10^2\).

5) In the case of the collapsed 3σ – 6σ halos (see Núñez-López et al. (2006)), the optical depth must increase by \(100 - 200\) times and the observational time would be reduced to a fraction of one hour for the NBBN model of Rauscher et al. (1994), and probably even the model of IBBN suggested by Lara (2007) with \([C]/[H] = 3 \cdot 10^{-13}\) could be detected, by taking into account that the enhancement of the CH fractional abundance during the collapse of the protocloud, leads to detectable fluctuations in the CMBR temperature. For this reason it is of great importance to do detail investigation of the non-linear stages of collapse at the first structure formation epochs.

6) As it was mentioned above, the first stars (PopIII) possibly appeared at \(Z \approx 20\), and significantly enriched the environments with heavy elements. In this case the relative abundance of \(^{12}\text{C}\) at \(Z = 19\) due to feedback can reach \([C]/[H] = 10^{-4}\) (Daigne et al. 2004), an abundance that is expected to be detected with modern radio telescopes.

To conclude, we would like to stress again that the optical depths in the rotational lines of the CH molecule from the first structures depend strongly on the models of NBBN and structure formation, and that in some cases these lines might be observable today, whereas for others it is not yet possible. In any case, this work emphasizes the need to search for signatures of these objects in order to find them or, at least, to put upper limits to constrain scenarios of formation and NBBN models.

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