PRIMORDIAL MOLECULES AND GRAVITATIONAL COLLAPSES

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Abstract. We analyze the formation of molecules based on carbon, nitrogen, oxygen and fluorine during the Dark Ages in two different contexts: the standard Big Bang nucleosynthesis model on the one hand and a particular, non-standard nucleosynthesis scenario on the other hand. The latter is particularly efficient in creating heavy nuclei. We also study, in these two different frames, the influence of the molecular H_2 and HD cooling functions on the gas temperature of a collapsing cloud.

1 Dark Ages chemistry of heavy elements

The cosmological gas hosted various chemical reactions and different molecules were created during the Dark Ages, the main ones being molecular hydrogen and HD. Heavy nuclei such as C, N, O or F were formed in very negligible amounts in the standard Big Bang nucleosynthesis model, because of the inexistence of stable elements with mass numbers 5 or 8 and because of the growing importance of the coulombian repulsion. For this reason, we expect molecules based on these elements to be produced in very small quantities. However, heavy nuclei can be efficiently synthesized in some non-standard nucleosynthesis models, in which small parts of the Universe have a high baryonic density, while most of the volume of the Universe is characterized by the usual, small baryon-to-photon ratio. We will here consider the particular non-standard nucleosynthesis scenario of Rauscher et al. (1994). This model is particularly efficient in creating heavy nuclei. In this scenario, the formation of such nuclei is a consequence of baryon density inhomogeneities, which induce local variations of the neutron-proton ratio. Heavy nuclei are then synthesized by neutron captures in neutron rich regions. In this particular nucleosynthesis case, the most abundant element is not hydrogen, but helium.

We compute the chemistry of H, D, He, Li, C, N, O and F from $z = 10^4$ to z = 10, using a large set of reactions that come mainly from the UMIST database (www.udfa.net) for the heavy elements C, N and O. We take the rates discussed in Puy et al. (2007) for the fluorine chemistry. We solve the complex set of differential equations governing the Dark Ages chemistry in the two distinct frames discussed above (we will call them standard and non-standard). Our results can be seen in Fig. 1. The main heavy molecules like CH, OH or NH and their respective molecular ions are created in amounts up to eleven orders of magnitude higher in the non-standard chemistry case. Globally, we obtain much lower abundances than in similar studies (e. g. Lipovka et al. 2007). We think that this is due, at least partly, to our much more extended reaction set.

2 Molecular cooling and gravitational collapses

Once primordial molecules are synthesized, they play a determining role in the formation of the first (Population III) stars. In particular, they are believed to be the only agent likely to cool down the primordial clouds undergoing gravitational collapses. We define the molecular thermal function Ψ_{mol} of a given molecule as the difference between its heating function Γ_{mol} (energy gain via radiative excitation of a rotational level followed by collisional deexcitation) and its cooling function Λ_{mol} (energy loss via collisional excitation followed by radiative deexcitation). For Ψ_{H_2} , we compute rotational level populations for levels up to J = 20 at each timestep and consider collisions of H₂ with H and He. We use the very recent collision rates of Wrathmall, Gusdorf & Flower (2007) for collisions with H, and Le Bourlot et al. (1999) for collisions with He. For the computation of Ψ_{HD} , the first eight levels are considered. We use the collision rates from Flower & Roueff (1999) for collisions with

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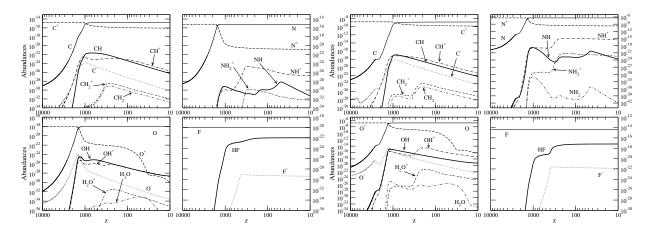


Fig. 1. Dark Ages chemistry of carbon, nitrogen, oxygen and fluorine. Left: Standard Big Bang chemistry. Right: Chemistry in the particular, non-standard model of Rauscher et al. (1994).

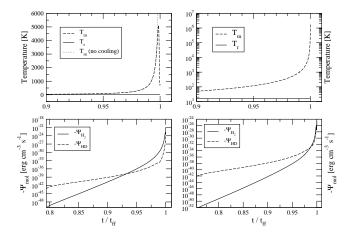


Fig. 2. Top: Evolution of the gas (T_m) and radiation (T_r) temperatures. Bottom: Evolution of Ψ_{H_2} and Ψ_{H_D} .

H, He and H₂. Fig. 2 shows the evolution of Ψ_{H_2} , Ψ_{HD} and the gas temperature T_m inside a collapsing $10^{10} M_{\odot}$ cloud. We use a 1D model of a perfectly homogeneous, spherical cloud. The left column shows the collapse in the case of the standard chemistry. We see that the cooling is dominated first by Ψ_{HD} . Then, when $T_m \sim 60 \text{ K}$, Ψ_{H_2} becomes dominant. The most interesting point is that after almost one free fall time, T_m starts to decrease, illustrating the efficiency of primordial molecules as cooling agent. The right column of Fig. 2 considers the same collapse, but this time in the non-standard chemistry scenario of Rauscher et al. (1994). Indeed, HD is more abundant in this case than H₂, and Ψ_{HD} could dominate the thermal properties of the collapsing gas. Unfortunately, Fig. 2 leads to the conclusion that the molecular cooling is less efficient in that case by a factor of the order of 2000. As a consequence, T_m never decreases.

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